Non equilibrium effects in fragmentation

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Abstract

We study, using molecular dynamics techniques, how boundary conditions affect the process of fragmentation of finite, highly excited, Lennard-Jones systems. We analyze the behavior of the caloric curves (CC), the associated thermal response functions (TRF) and cluster mass distributions for constrained and unconstrained hot drops. It is shown that the resulting CC’s for the constrained case differ from the one in the unconstrained case, mainly in the presence of a “vapor branch”. This branch is absent in the free expanding case even at high energies. This effect is traced to the role played by the collective expansion motion. On the other hand, we found that the recently proposed characteristic features of a first order phase transition taking place in a finite isolated system, i.e. abnormally large kinetic energy fluctuations and a negative branch in the TRF, are present for the constrained (dilute) as well the unconstrained case. The microscopic origin of this behavior is also analyzed.

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I. INTRODUCTION

The possibility of getting information about the thermodynamics of nuclear matter from the analysis of intermediate energies heavy ion collisions has triggered a lot of interest in this field. Starting from the pioneering work of the Purdue group, when for the first time a power law was used to fit the mass spectra resulting from highly excited nuclear systems and thus suggesting that a critical phenomena was taking place, it has open the study of a rather new branch of thermodynamics i.e the study of phase transitions (liquid-vapor) in finite systems \[1\].

One of the most challenging features that nuclear multi-fragmentation phenomena presents, is that signals of phase transitions of different orders can be extracted from experimental data. On one hand, the analogy between the nuclear force and a van der Waals interaction suggests that the nuclear equation of state should reproduce the main features that characterize a liquid-gas phase transition. Different indications of this kind of transition have been reported \[2\] \[3\]. On the other, signatures of a second order phase transition or critical behavior have been obtained assuming Fisher-like scaling relations for fragment distributions \[3\] \[10\]. Moreover, in recent works \[11\] \[12\] is suggested that the observed critical behavior is compatible with a first order phase transition, and it is due exclusively to finite size effects.

An important point to be kept in mind is that the above mentioned approaches to the fragmentation problem are based on descriptions where not only the concept of thermodynamical equilibrium, but also the macroscopic constraints imposed to the system play a relevant role. For example, several statistical descriptions of the nuclear multi-fragmentation process, e.g. the statistical multifragmentation model (SMM) \[13\] and the microcanonical Metropolis Monte Carlo model (MMMC) \[3\], employ the concept of a freeze-out volume inside of which the existence of a thermodynamical equilibrated ensemble of fragments is assumed. These statistical models have been widely used by the nuclear community in a successful manner to described some experimental observations. However, from the
experience gained in numerical simulations, such a concept as freeze-out volume, even as an approximation, does not seem to be completely correct. It is then important to study which kind of differences arise as a consequence of not assuming a finite volume scenario, as it is not \textit{a priori} evident that the evolution of a fragmenting system confined in a finite volume would produced the same macroscopic observable when compared with a non confined one, in which an expansive motion is present as an extra collective degree of freedom.

In previous works \cite{16,17} we have studied the fragmentation of a simple classical system where the dynamics is governed by a Hamiltonian with a two body interaction Lennard-Jones term. A microscopic description, employing molecular dynamics techniques, was used in order to adequately handle the possible presence of a non equilibrium behavior. It was shown that a fragmentation time can be defined, after which a certain degree of local equilibrium is achieved in the system. This fact allowed us to calculate a caloric curve for our expanding-fragmenting system, which is characterized by the absence of a vapor branch.

The aim of the present communication is to study how the restriction of a finite volume, and then the imposition of equilibration, affects some of the results obtained in the unconstrained case. We will show that one of the main effects is seen in the behavior of the caloric curve (CC). For the constrained system it clearly shows a vapor-branch, which is absent in the free expanding case. This behavior is a direct consequence of the presence of a confining volume, which destroys the velocity correlations that, in the case of the free expanding system, build up an expansive flux that acts as a heat sink. Nevertheless for both cases (at rather low densities for the constrained system) a local maximum and a loop in the CC can be seen. This feature can be associated with a negative branch in the corresponding thermal response function (TRF), that might signal a phase transition of first order. A gradual smoothing of the mentioned indicators is observed for the confined system at higher densities. Differences in fragment mass distributions are also reported and related to the microscopic origin of such behavior.

This paper is organized as follows. In Section \textit{II} we will describe the model used in our simulations. A brief review of the results already obtained for the unconstrained expanding
system is included. Section III is devoted to the study of the caloric curves. In Section IV we study possible choices for the freeze out volume for the constrained case. In Section V we calculate the thermal response functions and the kinetic energy fluctuations in order to signal the presence of possible phase transitions. A microscopic correlations study is performed in Section VI analyzing the results of two different clusterization algorithms. Finally, in Section VII, conclusions are drawn.

II. NUMERICAL SIMULATIONS

The system under study is composed by excited drops made up of particles interacting via a 6-12 Lennard Jones potential, which reads:

\[
V(r) = \begin{cases} 
4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} + \left( \frac{\sigma}{r_c} \right)^{12} + \left( \frac{\sigma}{r_c} \right)^{6} \right] & r \leq r_c \\
0 & r > r_c 
\end{cases}
\]  

(1)

We took the cut-off radius as \( r_c = 3\sigma \). Energies and distances are measured in units of the potential well (\( \epsilon \)) and the distance at which the potential changes sign (\( \sigma \)), respectively while the unit of time used is: \( t_0 = \sqrt{\frac{\sigma^2 m}{48\epsilon}} \). We integrated the set of classical equations of motion using the well known Verlet algorithm [14], taking \( t_{int} = 0.002t_0 \) as the integration time step. Initial conditions were constructed using the already presented method of cutting spherical drops composed of 147 particles out of equilibrated and periodic 512 particles per cell L.J. system [17].

A broad energy range was considered such that the asymptotic mass spectra of the fragmented drops for the unconstrained system changes from a "U shaped" pattern to an exponentially decaying one. Somewhere in between this two extremes a power law like spectra can be obtained.
A. Analysis of the unconstrained expanding case

For the sake of completeness we summarize in this section the main results obtained in previous work for the non-constrained fragmenting system (see [17] for details).

Due to the fact that we are dealing with a non-stationary process the determination of the time at which fragments are formed becomes one of the key ingredients in the analysis. To accomplish this task one can use a simple and intuitive cluster definition, that is based on correlations in configuration space: a particle \( i \) belongs to a cluster \( C \) if there is another particle \( j \) that belongs to \( C \) and \( |\mathbf{r}_i - \mathbf{r}_j| \leq r_{cl} \), where \( r_{cl} \) is a parameter called clusterization radius (In this work we used \( r_{cl} = r_{cut} = 3\sigma \)). The recognition algorithm introduced by this definition is known as minimum spanning tree (MST) fragment recognition method.

In [18] it was shown that a different recognition method, the Early Cluster Formation Model and its companion practical realization the so called Early Cluster Recognition Algorithm (ECRA), outperforms the MST clusterization algorithm in the sense that it finds the asymptotic fragmentation pattern in phase space at early stages in the evolution, when fragments are still not observables in configuration space. At that time the system still looks like a rather compact piece of excited matter. Instead of being defined through a proximity criteria, the ECRA fragments are associated with the set of clusters \( \{C_i\} \) for which the sum of the fragment internal energies attains its minimum value:

\[
\{C_i\} = \text{min} \{c_i | E_{\{C_i\}} = \sum_i E_{int}^{C_i} \}
\]

\[
E_{int}^{C_i} = \sum_i \left[ \sum_{j \in C_i} K_{j,c.m.} + \sum_{j,k \in C_i, j \leq k} V_{j,k} \right]
\]

where the first sum in (2) is over the clusters of the partition, \( K_{j,c.m.} \) is the kinetic energy of particle \( j \) measured in the center of mass frame of the cluster which contains particle \( j \), and \( V_{ij} \) stands for the inter-particle potential. We dub the partition found by ECRA as the most bound density fluctuation in phase space (MBDF) and we define as time of fragment formation \( (\tau_{ff}) \) the time at which the MBDF attain microscopic stability (see appendix for details). In this way \( \tau_{ff} \) is related to the time at which the systems switches from a regime
dominated by fragmentation to one in which the dominant decay mode is evaporation of light aggregates (mostly single particles) by the excited fragments. In this way the ECFM-ECRA outperforms the MST not only in terms of the time at which fragments are detected but also in it’s capability of unveiling the nature of fragmentation process. It shows that fragments are formed in phase space as a consequence of correlations in both q-p space.

Once the time of fragment formation is determined it is possible to calculate several properties of the system at fragmentation time. For this purpose the expanding system is decomposed in concentric shells and the mean radial velocity is calculated. It can be seen that the expansion is almost linear with the distance to the center of mass of the system, and that a local temperature can be defined as the fluctuations of the velocity around the local expansive collective motion. Moreover, the isotropical character of those fluctuations supports the idea that local equilibrium is achieved \[17\].

It is worth noticing that, on one hand at $\tau_{ff}$ most of the system is still interacting, and on the other the local temperature of the inner shells attain a rather constant value that can be consistently considered as the temperature of the system at fragmentation time. This can be seen in figure \[1\] where we show, for different energies, the dependence of the local temperature, $T_{loc}(r)$, and the local density, $\rho(r)$, as a function of the distance to the center of mass at fragmentation time.

**B. Analysis of the Constrained System**

In order to study the consequences of imposing a finite volume constraint to our system we used a spherical confining ‘wall’. The considered external potential behaves like $V_{wall} \sim (r - r_{wall})^{-12}$ with a cut off distance $r_{cut} = 1\sigma$, where it smoothly became zero along with its first derivative. A rather broad range of values for $r_{wall}$ were used.

Inside this potential, a highly excited drop was initialized in the way already described above and the corresponding equations of motion were integrated. Once the transient behavior was over we performed a microcanonical sampling of particle configurations every $5t_0$
up to a final time of $140000t_0$.

In this case the standard prescription for temperature calculation in the microcanonical ensemble was used, i.e. the kinetic energy ($K$) was related to the temperature of our $N$-particles system using:

$$T = \frac{2}{3(N - 1)} K$$

### III. CALORIC CURVES

One of the thermodynamics measurements that remains useful in the small system limit (hundred of particles) is the caloric curve, i.e. the functional relationship of the system temperature with its excitation energy.

The resulting caloric curve (CC) for the unconstrained system is displayed in Fig. 2a). In this figure circles denote the temperature of the system, already defined in Section II A, as a function of the energy. On the same figure a curve denoted by squares is also present, for this one the total kinetic energy, i.e. including both the fluctuations around the collective motion and the collective motion itself, is used instead. Of course this is not a temperature, just a fraction of the total kinetic energy, but it is then obvious that collective motion begins to be noticeable around a value of $E = 0$, and it becomes dominant at around $E = 2.\epsilon$.

Two main features are to be noticed, in first place the CC develops a maximum, and second the CC has no "vapor branch" but develops a rather constant behavior. These features are in contrast with the standard expectations inherited from the thermodynamics of infinite systems.

In Fig.3) we show the behavior of $T(E, \rho)$ for the constrained system (see also Fig.4a), where for the sake of clarity, we include just three different values of $\rho$).

For all density values a vapor branch is clearly observed. Moreover, comparing Fig.2(a) with Fig.3 and Fig.4a), it is clear that the vapor branch is due to the presence of the confining volume which inhibits the formation of radial collective motion that behaves like a heat
sink in the non constrained case. Inside the volume the emitted aggregates can do nothing but interact among themselves, and with the constraining wall, until thermal equilibrium is attained.

The effect of the boundaries on the CC is not important as long as the total energy in the system is small enough, and the expansive collective motion (in the unconstrained case) can be neglected. But this is not the case for highly excited finite systems, for which the presence of the constraining wall prohibits the formation of the expansive radial motion. For that range of energies the local equilibrium features that can be found in the fragmentation of the unconstrained system are replaced by global equilibrium ones when the dynamics is confined to finite volumes. This means that one has to be at least extremely careful if one intends to analyze expanding systems using confining volumes or any other model that rely on a global equilibrium hypothesis.

Another interesting feature to be notice in Fig.3) and Fig.4a) is the presence of a loop at the beginning of the gas rise in the CC for diluted enough systems. This back-bending behavior is gradually smeared out as the system density is increased. In Section V we will relate this to the behavior of the thermal response function of the system and in Section VI we will find that this can also be understood with the aid of the mass spectrum resulting from the MST and ECRA analysis.

IV. FREEZE OUT VOLUME APPROXIMATION

As was already shown, due to the intrinsic non-equilibrium character of the fragmentation process in the non-confined case, an assumption of local equilibrium (‘mounted’ over an expansive radial flux) instead of a global one has been found to be more appropriate. Accordingly, distributions of density and temperature, and not unique values, are necessary to described the system at fragmentation time in a rigorous way(see Fig.4). It is then not expected to find an exact mapping in the \((T, \rho)\) space between the constrained and
non-constrained dynamics.

Nevertheless if one insists on establishing such a comparison, two different criteria can be adopted in order to choose the appropriate volume for the constrained case (which we will call \( \textit{freeze-out volume}, V_{fo} \)). On one hand it can be seen from Fig.1) that at \( \tau_{ff} \) the local density value for the inner cells (where most of the mass is present at the time of fragment formation) remains rather constant (\( \rho \sim 0.08\sigma^{-3} \)) for the broad energy range presented in the figure. Accordingly, one can choose \( V_{fo} \) in order to attain such density value in the constrained case. This election, that could be considered as a ‘density-guided’ choice, corresponds to \( r_{\text{wall}} \sim 8\sigma \) and a \( \textit{freeze out} \) density value of \( \rho_{fo}^+ \sim \rho_0/10 \).

For the other hand a different approach can also be adopted looking at Fig.2a) and Fig.3a). It can be verified that for energy values where the onset of the fragmentation process occurs (\( -2\epsilon \leq E \leq 0\epsilon \)) the thermal energy in the expanding system is clearly lower than for the \( r_{\text{wall}} = 8\sigma \) case in the constrained case. In fact, similar temperatures can be found in the constrained case only for much diluted situations, i.e. for \( r_{\text{wall}} = 12\sigma \). In this sense, from a ‘temperature point of view’, a different \( \textit{freeze out} \) density \( \rho_{fo}^- \sim 0.02\sigma^{-3} \sim \rho_0/40 \) can be established.

As we mentioned above this ambiguity in the definition of a \( \textit{freeze out} \) volume (or density) is a consequence of trying to reproduce the behavior of an expanding fragmenting system using a global equilibrium scenario.

V. THERMAL RESPONSE FUNCTION

In recent works \([3,5,15]\) a lot of attention has been paid to the role played by the behavior of the specific heat (or more generally speaking: the thermal response function, \( TRF \)) as a signal of the occurrence of a phase transition in finite systems. Moreover, it has been shown (see \([3]\)) that the presence of a negative branch in the \( TRF \) can be related to a first order phase transition taking place in an isolated finite system. This kind of analysis can straightforwardly be performed over the systems under the current study, using the already
calculated CC and taking into account that the respective TRF’s can be calculated as:

\[ TRF = \left( \frac{\partial T}{\partial E} \right)^{-1} \]  \hspace{1cm} (3)

In Fig.2b) we show the TRF for the unconstrained system. Two poles can be seen. The first one \( (E \sim -0.5\epsilon) \) signals the entrance of the system into the multifragmentation regime, while the second one is related to the leveling off in the corresponding CC, and can be related to the increasing limit imposed by the strong flux to the ‘thermalization’ of the total available energy.

Fig.4b) shows the corresponding TRF for the constrained case. We include the curves for the two limiting cases discussed in Section IV as possible freeze out choices, i.e. \( \rho_{fo}^+ \) and \( \rho_{fo}^- \), and an intermediate \( \rho^0 \sim \rho_0/20 \) value \( (\rho_{fo}^- < \rho^0 < \rho_{fo}^+) \). We notice that two poles and a negative branch can be observed for the \( \rho_{fo}^- \) TRF curve. In this case we can relate the first pole with the onset of the transition, and the second one with the entrance in the gas phase, the energy distance between them being related to the associated latent heat. For \( \rho = \rho^0 \) it can be seen that the curve exhibits a qualitatively similar behavior, the distance between the two poles is just reduced. Nevertheless, for higher density cases, such as \( \rho_{fo}^+ \), the two poles merge into a single ‘singularity’ limited by finite-size effects. In that case, the TRF remains positive for all energies, showing a peak as a signature of the transition, as a consequence of the fact that the corresponding caloric curve does not display a loop but instead a simple change of slope (see next section for an analysis of this change of behavior).

Before leaving this section we would like to discuss, using an approach introduced in [15], the behavior of the fluctuations in the kinetic energy as an indicator of the occurrence of a phase transition in our finite system. In [15] it is shown that for an isolated and equilibrated system in which the total energy can be decomposed as: \( E = E_1 + E_2 \) the heat capacity can be calculated as:

\[ C \approx \frac{C_1^2}{C_1 - \sigma_1^2/T^2} \]  \hspace{1cm} (4)
where $C_1$ is the heat capacity associated with the subsystem-1, $\sigma_1$ is the fluctuation of the partial energy $E_1$, and $T$ the temperature of the system. In this context, the presence of poles and negative values in TRF’s can be associated to abnormally large fluctuations of the partial energy stored in subsystem-1, i.e. $\sigma_1^2 \geq C_1 T^2$, during the phase transition.

In Fig.5) we show, for the constrained case, the relative fluctuation, $A(E)$, for the kinetic energy defined as:

$$A(E) = N \frac{\sigma_K^2 |E|}{<K>|_E^2}$$

where $N$ is the number of particles in the system, and $<>$ stands for an average over the microcanonical sampling of configurations. We show the direct calculations using equation 5 for both, $\rho_f^+o$ and $\rho_f^-o$, and we also include the estimation of $A(E)$ derived for the respective CC’s in Fig.5). A rather good agreement can be seen between both ways of calculating this magnitude. In the same graph a reference level marks the canonical value for $A(E)$. As expected, for the appropriate range of energies, ‘unusually’ large relative fluctuations for the $\rho_f^-o$ case can be observed, while for the $\rho_f^+o$ case a local maximum, that does not exceed the canonical value can be seen. We postpone an analysis of this behavior until the next section, where we will study the properties of the system clusters.

We now try to extend the above performed analysis for the unconstrained system. In order to do that, we considered the central region (or core) defined by $r <= 6 \sigma$, and we calculated the total energy, $E_{core}$, and the number of particles $N_{core}$ that remains inside the core at fragmentation time. Binning the whole set of events according to these variables we can sample unconstrained fragmenting events in a pseudo-microcanonical way in what concerns core-quantities at $\tau_{ff}$. In Fig.6) we show the behavior of the relative fluctuation of the core kinetic energy, $A(E_{core})$, calculated using eq. 5 with $K = K_{core}$ and $N = N_{core} = 60 \pm 5$. In the same figure we include the canonical reference level. Even with a severe reduction of statistics imposed by the binning, a region of large fluctuations in $K_{core}$, for $N_{core}$ and $E_{core}$ fixed, can be easily recognized. This finding suggest that the 'large kinetic energy fluctuation signal', counterpart of the behavior observed for the corresponding CC
and TRF, can still be found for the expanding case.

VI. CLUSTER DISTRIBUTION

In previous sections we have analyzed our system studying thermodynamical features like the behavior of the CC and the TRF. In this part of the work we will focus our attention to a different aspect of the process, more directly related to microscopic correlations, that can be studied using the clusterization algorithms already introduced in Section II A.

Let us begin with the simple MST analysis. As this cluster recognition method is exclusively based on spatial correlations one expects for high density situations a big MST-cluster to be present. On the other hand, for lower densities a deviation from the U-shaped behavior in the mass spectra can be expected. As was already stressed, MST underestimates the number of clusters because it does not take into account the relative velocities of the cluster constituent particles. For unconstrained systems this effect was apparent when we considered the time of fragment formation, at this time the system was already fragmented in phase space, but in configuration space, a big cluster was still present. Due to the fact that the system was free to expand the asymptotic stage was such that MST converged to ECRA. But in the constrained case such an expansion is prohibited and then MST will not converge to ECRA.

Nevertheless, an interesting point to be notice is that the MST algorithm can still provide useful information about the limit imposed by the constraining finite volume to the formation of well defined fragments in configurational space because it reflects the size of the interacting subsystems present at a given time.

To further explore this we studied the behavior of the MST clusterization when applied to constrained systems at high energies. We observed that once we enter the ‘vapor-branch’, the spectra remain unchanged. In Fig. we show the obtained MST cluster distribution for four different densities at energies that situate the systems in the vapor-branch in the respective CC. It can be seen that the MST-spectra go from a U-shape up to an exponential
decaying behavior as the system density decreases. Notice that for densities around $\rho \sim \rho_{f0}$ a power-law like shape can be recognized. That means that from the spatial point of view the system admits, at least in principle, fragment configurations formed by well separated clusters of almost all possible sizes.

In Fig.8 we show the mean value of the size of the maximum MST-fragment as a function of the energy for the two densities taken as a reference. It can be seen that for the dense case, $\rho = \rho_{f0}^+$, the maximum fragment comprises almost all of the mass of the system irrespective of the value of the energy deposited in it. On the other hand for $\rho = \rho_{f0}^-$ the size of the biggest fragment decreases with increasing energy. This results support the idea that for the high density constrained case, no surfaces can be built in order to get small MST-fragments at high densities, whereas at low densities MST-fragments are well defined structures in configuration space and the surfaces appear.

We will now discuss the results obtained within the ECFM model. In Fig.9 we show the ECRA and MST mass distribution for the unconstrained system, both calculated at $\tau_{ff}$. We also show the same quantities calculated for the constrained case at densities $\rho = \rho_{f0}^+$ and $\rho = \rho_{f0}^-$.

First we can notice that for the dense constrained case MST always gives essentially the same U shaped curve, while the ECRA spectra show the usual transition from U shaped to exponentially decaying behavior. On the other hand, for the low density constrained case and the unconstrained case both the MST and ECRA results show such a transition.

It is interesting to note that when comparing the most energetic case the ECRA mass distributions corresponding to the constrained cases present a steeper slope than the corresponding to unconstrained situation (figures 9 (d), (h), and (l)). This happens as a direct consequence of the existence of boundaries. For the constrained cases the violent inter particle collisions, that are present at all times due to the reflections of particles with the constraining walls, destroy almost every correlation in phase space. On the other hand, for the unconstrained case the system develops a collective expansive motion which limits the ‘thermal’ component of the kinetic energy, allowing for the build up of well correlated den-
sity fluctuations in phase space, i.e. ECRA-clusters (note also that while the ECRA clusters are microscopically stable for the unconstrained case, the ones for the constrained system are not). It is in this regime where the differences between a local equilibrium picture and a global one become important.

As long as the collective expansive energy in the free case can be neglected ($E \lesssim 0.5\epsilon$) the ECRA spectra present a rather similar shape for the three shown cases. Moreover, a clear signature of a first order phase transition can be recognized in the shape of the ECRA spectra noticing the simultaneous presence of a ‘liquid-phase’ (mass fragments $m \sim 30$) and a ‘gas-phase’ (mass fragments $m < 10$) for $0.1\epsilon \leq E \leq 0.4\epsilon$.

This findings clarify the shapes of the corresponding CC. For the dense constrained system, $\rho_{\bar{f}_0}$, we have a big configurational MST-cluster all the time, inside of which an (unstable) ECRA partition can be defined that exhibits features expected for a first order phase transition. The fact that the whole system is strongly interacting (there are no spatial surfaces dividing ECRA-phases) is responsible of the reduction of the back-bending behavior in the corresponding CC and the lack of strong kinetic energy fluctuations. For the more dilute case, $\rho_{\tilde{f}_0}$, the system is capable of ‘reproduce’ phase space surfaces (at least at some degree) in configurational space and the mentioned signals start to be noticeable.

An extra support to the idea that fragmentation do take place in phase space not only for the free expanding system (see [16]) but also for the constrained case can be gained if we remove the external ‘wall’ potential and let the system expand. In Fig.10 we compare the asymptotic spectra resulting from such a process of removal of the constraints, with the ECRA one obtained with boundaries for $\rho_{\tilde{f}_0}$ and $\rho_{\bar{f}_0}$ cases at $E = 0.4\epsilon$ and $E = 0.7\epsilon$. A quite remarkable agreement can be found. The fact that this agreement is better for lower densities reflects that different degree of spatial-fragmentation is achieved at different densities. In this way, for $\rho_{\tilde{f}_0}$, the differences in both spectra (slight suppression of intermediate mass fragments favoring bigger clusters) can be understood as consequence of an aggregation-like process occurring during the early expansive stage due to the strong interacting nature of the system.
In Section V we showed for the confined system that the diverging behavior of the TRF is related to abnormally large fluctuations of the kinetic energy. In order to understand the origin of those fluctuations we show in Fig. [11] the system kinetic energy $K$ and the mass of the biggest ECRA-cluster as a function of time for $\rho = \rho_f$ at $E = 0.4e$. Also the mass of the biggest MST-cluster is shown. It is clearly seen that the first two quantities are well correlated while the MST biggest cluster is not. This indicates that from a microscopic point of view the systems is sometimes mainly liquid (big ECRA biggest cluster) and others it is mainly vapor (small ECRA biggest cluster). This phase alternation is the kind of coexistence expected for finite system (see [13]).

VII. CONCLUSIONS

In this work we have presented a complete analysis of Caloric Curves, Thermal Response Functions and MST and ECRA fragment distributions for constrained and unconstrained excited liquid drops. We have shown that the effect of constraints is quite important, and that its main result is to allow the system to reach thermal equilibrium. In particular the Caloric Curves for constrained cases show a vapor branch which is clearly an ‘equilibrium effect’ that is not present for unconstrained systems.

We have also verified, studying the behavior of ECRA-cluster mass distributions, that fragmentation does occur in phase space in all the studied cases. Moreover, phase coexistence can be found in all ECRA spectra at appropriate energies (we have shown that the ECRA fragments in constrained systems correspond closely to the MST asymptotic clusters when the constraints are removed. This reinforces the validity of the ECFM-ECRA approach to study fragmentation phenomena occurring in finite volumes).

It is interesting to notice that for the constrained case, as the system density is increased, the expected signals of a first order phase transition in the CC, TRF and kinetic energy fluctuations are gradually smoothed, and eventually disappear. This can be associated to the fact that at low densities ”internal surfaces” can be developed in the constrained
system allowing the transition to be traced in configurational space (i.e. MST clusters are formed reflecting the fact that well separated aggregates appear in coordinate space). Such a feature is not possible in the dense case, all of the time the system is composed by a big configurational cluster that comprises more than 95\% of the total mass.

Moreover for the constrained case, a relation between the fluctuations in size of the maximum ECRA-fragment and the kinetic energy fluctuations was established. As a consequence, the presence of abnormally large fluctuations in the system kinetic energy could directly be linked with a phase coexistence phenomenon taking place in a finite system.

As a final remark we want to emphasize that, even some similarities can be found between the behavior of low density constrained systems and unconstrained ones at low energies, such a comparison fails at and above the energy that corresponds to the onset of the fragmentation process, i.e. when the collective radial modes begin to drive the evolution of the system.

As we mentioned, the role of this collective motion is to behave as a heat sink, precluding the system from developing a vapor branch, and freezing the most bound density fluctuations in phase space allowing them to become the asymptotic clusters. This is why a ‘local’ equilibrium picture, and not a ‘global’ one, is necessary to describe the fragmentation process correctly, i.e. taking into account the effects of the radial flux. This teaches us that when dealing with fragmentation phenomena of the kind appearing in nuclear multifragmentation, caloric curves which display vapor branches should be taken with caution, and consequently the results obtained from models that display such a feature should be at least critically reexamined.

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A. Appendix

Once the clusters have been calculated using the ECFM we have to determine the time at which the fragmentation is over and the systems enters an evaporation regime (i.e the fragmentation pattern is formed and the fragments undergo a simple evaporation process). We will then define the time of fragment formation to that time at which the MBDF attain microscopic stability. This property of the clusters has been calculated using what we call the Short Time Persistence, in which we calculate the stability of MBDF against evaporation and coalescence. We define the time of stabilization in the following way: Given a configuration resulting from the ECRA analysis at a given time \( t \) we analyze the microscopic stability of each fragment \( C_i^t \) of size \( N_i^t \) by searching on all the fragments \( C_j^{t+dt} \) present at time \( t + dt \) for the biggest subset \( N_{\text{max}}^{t+dt}_i \) of particles that belonged to \( C_i^t \). We then assign to this fragment a value \( STP_d = \frac{N_{\text{max}}^{t+dt}_i}{N_i^t} \). In this way we are taking into account what we call the “evaporation process”. We also have to take into account that there can be some realization for which cases the \( N_{\text{max}}^{t+dt}_i \) does not constitute a subset of the original cluster \( C_i^t \) but is embedded in a bigger fragment of mass \( N_i^{t+dt} \). We include this effect by defining \( STP_i = \frac{N_{\text{max}}^{t+dt}_i}{N_i^{t+dt}} \) (with \( i \) standing for inverse). Finally the Short time persistence reads:

\[
STP(t, dt) = \left\langle \left\langle \left[ \frac{STP_d(t, dt) + STP_i(t, dt)}{2} \right] \right\rangle \right\rangle_m e^{(6)}
\]

where \( \langle \ldots \rangle_m \) is the mass weighted average over all the fragments with size \( N > 3 \). And \( \langle \ldots \rangle_e \) is the average over an ensemble of fragmentation events at a given energy \( E \).

A reference value for \( STP(t, dt) \) can be obtained considering that the fragments undergo only a simple evaporative process. In this way we say that when \( STP \) reaches this reference value the system goes from fragmentation to evaporation. We call this time \( \tau_{ff} \).
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FIGURES

FIG. 1. In the higher figure: local density at the initialization step (empty symbols) and local density at fragmentation time (solid symbols) as a function of the center of mass distance. In the lower figure: local temperature profile at fragmentation time as a function of the center of mass distance. Circles denote $E = 0.0\epsilon$, squares denote $E = 0.5\epsilon$, up-triangles denote $E = 0.7\epsilon$, diamonds denote $E = 0.9\epsilon$, and left-triangles denote $E = 1.2\epsilon$.

FIG. 2. In figure (a): Caloric curve calculated for the expanding system (solid circles). The empty squares correspond to an estimation of a ‘fake-temperature’ that does not take into account in a proper way the collective motion and is calculated simply as a fraction of the total kinetic energy (see text for details). Figure (b) shows the associated thermal response function.

FIG. 3. Temperature of the constrained system as a function of its energy and density.

FIG. 4. Caloric curve for the constrained system, figure (a), and the respective thermal response functions, figure (b), for three different densities: $\rho = \rho_{f_o}$, $\rho^0_{f_o}$, and $\rho^+_{f_o}$ (circle, triangle, square symbols in figure (a), and full, dashed, dotted-dashed lines in figure (b), respectively)

FIG. 5. Relative kinetic fluctuation, $A(E)$, for the constrained case calculated for different densities, as a function of the total energy. The symbols correspond to direct calculations for $\rho = \rho^+_{f_o}$ (empty squares) and for $\rho = \rho^-_{f_o}$ (solid circles). The lines correspond to $A$ estimations using the caloric curve (solid-line for $\rho = \rho^-_{f_o}$, and dashed-line for $\rho = \rho^+_{f_o}$). The dashed-dotted line shows the canonical expectation value for $A$.

FIG. 6. Relative kinetic energy fluctuation, for the non constrained system, as a function of the core-energy. The calculation includes only events with $N_{core} = 60 \pm 5$ particles inside the core.

FIG. 7. MST mass distribution calculated for the vapor-branch of constrained systems of densities: $\rho = 0.08\sigma^{-3}(\rho^+_{f_o})$, $0.035\sigma^{-3}$, $0.02\sigma^{-3}(\rho^-_{f_o})$, and $0.01\sigma^{-3}$ are shown in figures (a), (b), (c), and (d) respectively.
FIG. 8. Mean value of the mass of the biggest MST-cluster for the constrained case. Circles denote $\rho = \rho_0^+$, and triangles $\rho = \rho_0^-$. 

FIG. 9. ECRA (solid circles) and MST (empty squares) mass spectra calculated at fragmentation time $\tau_{ff}$. The first column corresponds to the free expanding case, the others to the $\rho = \rho_0^-$ and $\rho = \rho_0^+$ confined cases respectively. The considered system energies were: $E = -0.5\epsilon$, $E = 0.0\epsilon$, $E = 0.5\epsilon$, $E = 1.2\epsilon$, in figures (a)-(d) for the free expanding case, and $E = -0.2\epsilon$, $E = 0.1\epsilon$, $E = 0.4\epsilon$, $E = 1.2\epsilon$ in figures (e)-(f) and (i)-(l) for the constrained cases.

FIG. 10. Asymptotic mass distribution after the ‘wall’ removal (empty squares) and ECRA spectra calculated within boundaries (solid circles) for densities $\rho = \rho_0^+$ (first raw), and $\rho = \rho_0^-$ (second raw). Figures (a) and (c) corresponds to $E = 0.4\epsilon$, while (b) and (d) to $E = 0.7\epsilon$.

FIG. 11. In figure (a), the system kinetic energy is shown as a function of time for the constrained case at $\rho = \rho_0^-$ and $E = 0.4\epsilon$. The temporal dependence of the mass of the biggest ECRA and MST clusters are shown in figures (b) and (c) respectively.
\[ \rho_{\text{loc}}(\sigma - 3) \]

\[ T_{\text{loc}}(\epsilon) \]

\[ r(\sigma) \]
