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Microscopic Dynamics of Small Fragmenting Systems

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We calculate the Caloric Curve of fragmenting drops of Lennard Jones particles, defined as the temperature of the system at fragmentation time. We show how to calculate the time of fragment formation, and the temperature at this time. We explore the role played by the collective motion. The competition between the collective radial, ordered, motion and the intrisic, chaotic, motion is analyzed using the Maximum Local Lyapunov Exponent.

1. Introduction

We study fragmentation of excited drops formed by $N = 147$ particles interacting via a 6-12 Lennard Jones (L.J.) potential truncated at $r_{co} = 3\sigma$. Energy and distance are measured in units of ϵ, the potential depth and σ, distance at which the LJ potential changes sign. The unit of time is: $t_0 = \sqrt{\sigma^2 m/48\epsilon}$. The initial configurations are constructed by cutting a spherical drop from a thermalized, periodic, LJ system with $N = 512$ particles per cell. We studied a broad energy range, $-2.4\epsilon \leq E \leq 2.2\epsilon$, which result in different fragmentation patterns, from U shaped (low energy) to an exponentially decaying (high energy), see [1].

We focus on the calculation of the Caloric Curve (CC) and the analysis of the role of the collective (radial expansion) degree of freedom. We show that it is possible to calculate the time at which the fragments are formed, we then define CC as the temperature of the system at fragmentation time. We show that the fragmenting system achieves some degree of local equilibrium at this time, allowing us to define a "local temperature".

2. Time scales of fragment formation and emission

We now focus on the determination of the times of fragment formation and emission. We use two fragment recognition algorithms , [2]. In the simplest one, MST, a set of particles $i, j, k, \ldots$ belong to a cluster C if: $\forall\ i \in C\ , \exists\ j \in C\ /\ |\mathbf{r}_i - \mathbf{r}_j| \leq R_{cl}$, with $\mathbf{r}_i$ and $\mathbf{r}_j$ the positions of the particles and R_{cl} is the clusterization radius, $R_{cl} = 3\sigma$.

On the other hand, the Early Cluster Formation Model (ECFM) [3], states that: clusters are those that define the most bound partition of the system, i.e. the partition $(\{C_i\})$

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that minimizes:

$$E_{\{C_i\}} = \sum_i \left[\sum_{j \in C_i} K_j^{cm} + \sum_{j,k \in C_i} V_{j,k} \right] \quad (1)$$

where the first sum is over the clusters of the partition, and K_j^{cm} is the kinetic energy of particle j measured in the center of mass frame of the cluster which contains particle j. The algorithm (ECRA) devised to achieve this goal is based on an optimization procedure in the spirit of simulated annealing[3].

Furthermore, we have studied the microscopic stability of the clusters, [1] and we define two different time scales: a "fragment formation time" $\tau_{ff}(E)$ related to the ECRA partition differing from the asymptotic partition by an evaporation-like process, and a "fragment emission time" τ_{fe} when the MST partition does. For all energies $\tau_{ff}(E) \ll \tau_{fe}(E)$ and i at $\tau_{ff}(E)$ biggest MST cluster contains more than half the total mass of the system.

3. Effective temperatures and caloric curve

Being the radial collective velocity position dependent, we divide our drops in concentric spherical regions, centered in the c.m of the system, of width $\delta r = 2\sigma$. We define the mean radial velocity of region i as: $v_{rad}^{(i)}(t) = \frac{1}{N_i(t)} \sum_{ev} \sum_{j \in i} \frac{\mathbf{v}_j(t) \cdot \mathbf{r}_j(t)}{|\mathbf{r}_j(t)|}$ where the first sum runs over the different events for a given energy, the second over the particles j that belong, at time t, to region i; $\mathbf{v}_j$ and $\mathbf{r}_j$ are the velocity and position of particle j. $N_i(t)$ is total number of particles belonging to region i in all the events. We then define the local temperature $T_{loc}^{(i)}$:

$$T_{loc}^{(i)} = \frac{2}{3} \frac{1}{N_i} \sum_{j \in i} \frac{1}{2} m \left(\mathbf{v}_j - \frac{v_{rad}^{(i)} \cdot \mathbf{r}_j}{|\mathbf{r}_j|} \right)^2 \quad (2)$$

This conjecture of local equilibrium, is supported by the fact that velocity fluctuations in the radial and tangential directions are of the same order.

In Fig. 1 we show, the "Extended Caloric Curve", (ECC) which encompasses the solid-like phase (region I), the liquid-like phase (region III), the associated phase transition (region II) [4], and the region of evaporation and multifragmentation (region IV).

In region IV we plot the local temperature averaged over the three inner most regions at τ_{ff}. We can see from Fig.1 that the local temperature at τ_{ff} is quite independent of the total energy of the fragmenting system.It slowly decreases for higher energies. This behavior can be traced to the presence of the collective expansion which behaves as a heat sink.We've found that the temperature of the system at τ_{ff} is the same as the temperature of the medium size fragments both at fragmentation time and at assymptotic times.

4. The Maximum Local Lyapunov Exponent

The Maximum Lyapunov Exponent (MLE), is a measure of the sensitivity of the system to initial conditions and gives an idea of the velocity at which the system explores the available phase space. Given two very close initial conditions in phase space (i.e. they

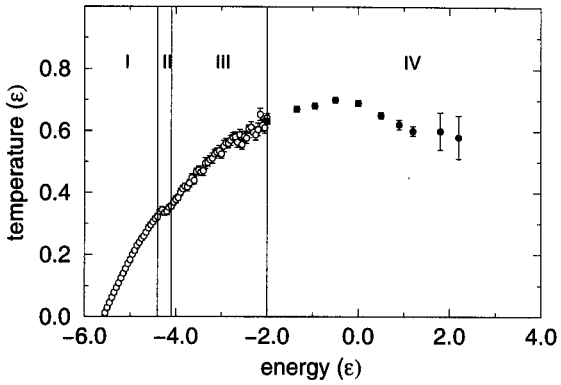

Figure 1. Extended Caloric Curve (see text for details)

differ at $t = 0$ a small amount d_0) , if the corresponding trajectories diverge exponentially, the MLE $\hat{\lambda}$ is given by the following relation : $\frac{\partial d}{\partial t}(t) = \hat{\lambda} d(t)$.

$d(t)$ is given by $d(t) = \left(\sum_{i=1}^{N}[a(\mathbf{r}_1(t) - \mathbf{r}_2(t))^2 + b(\mathbf{p}_1(t)) - \mathbf{p}_2(t))^2]_i\right)^{1/2}$, with $\mathbf{r}, \mathbf{p}$ the positions and momenta of N particles at time t. Indices '1' and '2' refer to the two trajectories. a, b are two arbitrary parameters which express the fact that the LE are independent of the particular metrics in phase space. We took $a = 0, b = 1/m$, where m is the mass of the particles.

The calculation of the MLE is as follows, after a time step τ we re-scale $d(\tau) = d_1$ to d_0 in the maximum growing direction and save the quantity $ln[d_1/d_0]$. Repeating the procedure at every time step τ, the MLE is defined as:$\lambda = \lim_{n\to\infty} \frac{1}{n\tau} \sum_{i=1}^{n} ln \left|\frac{d_i}{d_{i-1}}\right|$. We then define a Maximum Local Lyapunov Exponent (MLLE) associated with the i^{th} interval of size $N_i\tau$ as:

$$\lambda_i' = \frac{1}{N_i\tau} \sum_{j=i}^{i+N_i} ln \left|\frac{d_j}{d_{j-1}}\right| = \frac{1}{N_i\tau} ln \left|\frac{d_{i+N_i}}{d_i}\right| \tag{3}$$

with N_i finite. Because the system we analyze is characterized by its macroscopic state (i.e. the energy), we prepare an ensemble of initial points from which, after performing the above mentioned steps, we calculate $\lambda_i = < \lambda_i' >_e$ with $<>_e$ denoting the average over the ensemble of main points.

In fig. 2 we plot the MLLE as function of the energy at three relevant times. At $t = 2t_0$, the MLLE is an increasing function of the energy because the drop has had not enough time to develop the collective radial motion. We also show the MLLE at $t = 20t_0$ and at $t = 150t_0$. For both energies, the MLLE displays a maximum in the region between $E = -2.0\epsilon$ and $E = -1.3\epsilon$. and then decays for higher energies. In this

energy region the evolution of the system is dominated by the presence of a rather big fragment encompassing more than 80% of the mass of the original system.

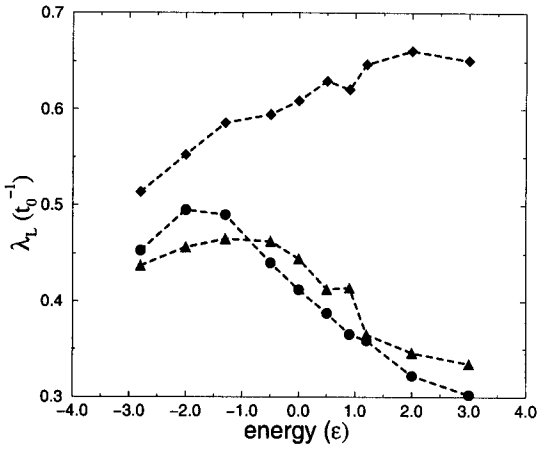

Figure 2. Lyapunov exponents as a function of the energy at relevant times, $t = 2t_0$ (diamonds), $t = 20t_0$(circles) and $t = 150t_0$ (triangles)

5. Conclusion

The fragmentation process can be divided in three stages. From $t = 0$ to $t = \tau_{ff}(E)$ the radial flux and density fluctuations in phase space develop. By the end of this stage the asymptotic fragments are already formed according to the ECFM model although most of the mass of the system is still interacting and forming a big MST cluster. From $\tau_{ff}(E)$ to $\tau_{fe}(E)$, the fragments separate in configurational space. Finally, $t > \tau_{fe}$, is the free expansion stage. The resulting ECC displays in the fragmentation regime a plateau followed by a monotonous, slow, decrease. Moreover, the behavio of the MLLE indicate that the system evolves from a highly chaotical early stage into a more regular one, which suggests a chaos to order transition.

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