Extended Gibbs ensembles with flow

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A recently proposed [Ph. Chomaz, F. Gulminelli, and O. Juillet, Ann. Phys. (Paris) **320**, 135 (2005)] statistical treatment of finite unbound systems in the presence of collective motions is applied to a classical Lennard-Jones system, numerically simulated through molecular dynamics. In the ideal gas limit, the flow dynamics can be exactly recast into effective time-dependent Lagrange parameters acting on a standard Gibbs ensemble with an extra total energy conservation constraint. Using this same ansatz for the low-density freeze-out configurations of an interacting expanding system, we show that the presence of flow can have a sizable effect on the microstate distribution.

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I. INTRODUCTION

The thermodynamics of isolated finite unbound systems cannot in general be associated with a stationary process. In condensed matter physics, cluster dissociation induced by photoionization [2–5] or charge transfer collisions [6,7] cannot be studied without properly accounting for the time window of the experiment [2]. Going down to the femto scale, the thermodynamic properties of nuclear systems can be accessed only through collisions [10]. It has been suggested [2,3,6] that the thermodynamics of the liquid-vapor phase transition can be relevant in explaining the cluster evaporation process. The connection with equilibrium statistical mechanics can be achieved by introducing the concept of an evaporative ensemble [8,9] with a time-dependent temperature.

Conversely, in the nuclear collision case, the time scales can be so short that the reaction and decay channels cannot be decoupled, collective flows appear, and the statistical equipartition hypothesis breaks down [11]. If in the Fermi energy regime and in the associated multifragmentation phase transition these collective flows may be only a perturbation in the global energetics, this is not true for heavy ion collisions as performed at the Schwerionen-Synchrotron (SIS) at energies (between 0.2 and 2 GeV/nucleon), where they are likely to influence light cluster formation by coalescence [12]. In the ultrarelativistic regime, the ordered and disordered motions become comparable in magnitude [23], and collective flows are believed to play an essential role in the characteristics of the transition to the quark-gluon plasma observed in the Relativistic Heavy Ion Collider data [13–15]. In particular, correlations and recombination of thermalized quarks from a collectively flowing deconfined quark plasma are supposed to be the dominant mechanism for soft-hadron production [13,16].

In all these very different physical situations, the huge number of available decay channels and the general complexity of the systems under study clearly call for a statistical treatment. However, the time dependence of the process makes the definition of statistical concepts like statistical ensemble, temperature, pressure, etc. unclear [17,18]. If it is intuitively recognized that the presence of incomplete equilibration and collective flows may be treated in a statistical framework introducing extra constraints [19], the procedure is not necessarily unique.

The inclusion of collective motion in the form of a radial or elliptic flow in equilibrium models has been treated by different authors [1,20–25]. The most widespread approach is to suppose a full decoupling between intrinsic and collective motion and assume for the expanding system a standard Gibbs equilibrium in the local rest frame [23,26]. The quality of this assumption obviously depends on the degrees of freedom and energy regime under study. Concerning heavy ion collisions, this assumption may be justified in the Fermi energy regime because of the limited energy percentage associated with directed motion [10], and in the ultrarelativistic regime by the empirical success of hydrodynamical models [15]. Some attempts have, however, been made to explicitly include flow in the statistical treatment. Limiting ourselves to classical systems of interacting constituents treated as elementary degrees of freedom, the empirical treatment of flow in Ref. [20] has been shown not to modify the correlation properties of the system. However, other empirical approaches [21,22] predict that the presence of flow should lead to a violation of statistical equilibrium weights, with a trend toward more unbound configurations. Experimental data in the nucleonic regime suggest that the influence of collective motion on the partitioning in the system may strongly depend on the deposited energy [27,28].

In this paper, we address the generic statistical mechanics problem of the definition of a statistical ensemble in the presence of a collective flow. The general formalism has been developed elsewhere, and applications were given in the canonical ensemble [1]. However, in the physical cases of interest the expanding system is isolated, and a microcanonical description is in order. We will use the example of a classical Lennard-Jones system [29] to evaluate some chosen observables for a statistical isolated system subject to a radial flow. Molecular dynamics simulations on the same system have already shown that flow enhances partial energy fluctuations [30] and at the same time can act as a heat sink [31,32],

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cooling the system and thus preventing it from reaching high temperatures. In this paper, we will show that, if flow is introduced as an extra constraint in the framework of an information theory approach, it can also act as a heat bath. Indeed, the partial relaxation of the microcanonical constraint, of an ensemble with conserved energy, allows the isolated system to explore a larger configuration space.

II. TIME-DEPENDENT GIBBS ENSEMBLES

The general formalism of the time-dependent Gibbs ensemble has been developed in a previous paper [1], and in this section we recall the main results relevant to the specific case of the dynamics of the expansion.

Flow naturally appears in the statistical picture [33,34] as soon as we introduce constraints which are not constants of motion. Consider an isolated physical system characterized by a finite spatial extension $\langle R^2 \rangle$ at a given time t_0. Introducing the density matrix $\hat{D}=\Sigma_{(n)}|\Psi^{(n)}\rangle p^{(n)}\langle\Psi^{(n)}|$, the minimum biased microstate probability distribution $p^{(n)}$ is defined by

$$\hat{D}_{\lambda_0}(t_0) = \frac{1}{W_{\lambda_0}(E)} \exp(-\lambda_0 \hat{R}^2)\, \delta(E-\hat{H}), \tag{1}$$

where $\hat{H}$ is the Hamiltonian, λ_0 is a Lagrange multiplier constraining the finite size, and

$$W_{\lambda_0}(E) = \sum_{(n)} \exp(-\lambda_0 R_n^2)\, \delta(E-H_n) \tag{2}$$

is the associated density of states or partition sum. The dynamical evolution of Eq. (1) at times $t>t_0$ is obtained from the Liouville equation $\partial_t \hat{D}=-i/\hbar[\hat{H},\hat{D}]$ [1], or equivalently from the time evolution of the constraint. In the Heisenberg representation,

$$\hat{R}^2(t) = e^{-i\Delta t\hat{H}} \hat{R}^2(t_0) e^{i\Delta t\hat{H}} = \hat{R}^2(t_0) + \sum_{p=1}^{\infty} \frac{(\Delta t)^p}{p!} \hat{B}^{(p)}, \tag{3}$$

where $\Delta t=(t-t_0)$ and the $\hat{B}^{(p)}$ operators are defined by the recursive relation

$$\hat{B}^{(p)} = -\frac{i}{\hbar}[\hat{H},\hat{B}^{(p-1)}], \quad \hat{B}^{(0)} = \hat{R}^2. \tag{4}$$

The time dependence of the process can therefore be recast in terms of an (*a priori* infinite) number of extra constraints $\hat{B}^{(p)}$. In the simplified case of a system of noninteracting identical particles

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m}, \tag{5}$$

the series reduces to the two operators

$$\hat{B}^{(1)} = -\frac{i}{\hbar}[\hat{H},\hat{R}^2] = -\sum_{i=1}^{N} \frac{1}{m}(\hat{\vec{p}}_i \cdot \hat{\vec{r}}_i + \hat{\vec{r}}_i \cdot \hat{\vec{p}}_i), \tag{6}$$

$$\hat{B}^{(2)} = -\frac{i}{\hbar}[\hat{H},\hat{B}^{(1)}] = \sum_{i=1}^{N} \frac{2\hat{p}_i^2}{m^2}. \tag{7}$$

Then the exact density matrix is given at any time $t>t_0$ by

$$\hat{D}_{\lambda_0}(t) = \frac{\delta(E-\hat{H})}{W_{\lambda_0}(E,t)} \exp \sum_{i=1}^{N} \left(-\beta(t)\frac{\hat{p}_i^2}{2m} - \lambda_0 \hat{r}_i^2 + \frac{\nu(t)}{2}(\hat{\vec{p}}_i \cdot \hat{\vec{r}}_i + \hat{\vec{r}}_i \cdot \hat{\vec{p}}_i) \right) \tag{8}$$

with

$$\beta(t) = \frac{2\lambda_0}{m}(\Delta t)^2, \quad \nu(t) = \frac{2\lambda_0}{m}\Delta t. \tag{9}$$

The diabatic evolution of an isolated initially constrained freely expanding system can then be described as a generalized Gibbs equilibrium in the local rest frame,

$$\hat{D}_{\lambda_0}(t) = \frac{\delta(E-\hat{H})}{W_{\lambda_0}(E,t)} \exp \sum_{i=1}^{N} -\beta(t)\frac{[\hat{\vec{p}}_i - mh(t)\hat{\vec{r}}_i]^2}{2m}. \tag{10}$$

Comparison with the exact solution Eq. (8) shows that the Hubble factor is linearly decreasing in time, $h=\Delta t^{-1}$.

These equations show that radial flow is a necessary ingredient of any statistical description of unconfined finite systems in the presence of a continuum; on the other hand, if a radial flow is observed in the experimental data, this formalism allows one to associate the flow observation with a distribution at a former time when flow was absent. This initial distribution corresponds to the standard description of an ideal gas in a confining harmonic potential. In this case, the infinite information which is *a priori* needed to follow the time evolution of the density matrix according to Eq. (3) reduces to the three observables $\hat{r}^2$, $\hat{p}^2$, and $\hat{\vec{r}}\cdot\hat{\vec{p}}+\hat{\vec{p}}\cdot\hat{\vec{r}}$. Indeed, these operators form a closed Lie algebra, and the exact evolution of $\hat{D}_{\lambda_0}$ preserves its algebraic structure. This treatment can be easily extended to nonisotropic flows [1] by introducing an initially deformed spatial distribution.

It is easy to see that Eq. (8) is still exact for an interacting system, if the density is low enough that interactions can be modeled as purely local interactions $\hat{v}_{12} \propto \delta(\hat{\vec{r}}_1 - \hat{\vec{r}}_2)$, as in the Boltzmann collision integral. If the interactions are nonlocal at the initial time t_0, this simple solution is not exact any more and higher-order operators play a role. Considering a finite-range two-body interaction $\hat{V}=\Sigma_{ii'}V(|\hat{\vec{r}}_i - \hat{\vec{r}}_{i'}|)$, we can see that the first-order correction in time to the static problem $\hat{B}^{(1)}$ is identical to the result for the ideal gas problem Eq. (6), while already at the second order $\hat{B}^{(2)}$ contains an additional term

$$\hat{B}^{(2)} = \sum_{i=1}^{N} 2\frac{\hat{p}_i^2}{m^2} - \sum_{ii'} \frac{1}{m}\hat{r}_{ii'}\vec{\nabla}V(\hat{r}_{ii'})$$

where $\hat{r}_{ii'}=|\hat{\vec{r}}_i - \hat{\vec{r}}_{i'}|$. In the case of a harmonic interaction the $\hat{B}^{(p)}$ operators only contain quadratic terms $\Sigma_i \hat{p}_i^2$, $\Sigma_{ii'}\hat{r}_{ii'}^2$, and

$\Sigma_{ii'}\hat{r}_{ii'}\cdot\hat{p}_{ii'}$, with $\hat{p}_{ii'}=\hat{\vec{p}}_i-\hat{\vec{p}}_{i'}$. In this case the time evolution can be taken into account by a suitable time-dependent temperature and the introduction of a radial flow.

For any other interaction $\hat{B}^{(2)}$ modifies not only the temperature but also the two-body interaction and an analytical solution is not possible. If interactions are short ranged and the unbound system evolves in the vacuum, a time will exist when the constituents (particles or clusters) cease to interact, entropy saturates, and the different observables reach their asymptotic value. This time is known in the literature as the freeze-out time. If at this time the system can be treated statistically, the succeeding evolution will be ruled by the ideal gas equations developed above. As a first-order approximation, we can therefore consider the statistical ansatz at the freeze-out time:

$$W_{\tilde{\beta}\tilde{\lambda}\tilde{h}}(E)=\sum_{(n)}\exp\left(-\tilde{\beta}\sum_{i=1}^{N}\frac{1}{2m}(\vec{p}_{in}-\tilde{h}m\vec{r}_{in})^2-\beta V_n-\tilde{\lambda}R_n^2\right)\delta(H_n-E), \tag{11}$$

where the sum runs over the microstates (n) of the phase space, V is the two-body interaction, and $\tilde{\beta},\tilde{\lambda},\tilde{h}$ are Lagrange parameters imposing given values for the average thermal energy, mean square radius, and local collective radial momentum at freeze-out through the associated equations of state

$$\langle E_{th}\rangle=-\frac{\partial W_{\tilde{\beta}\tilde{\lambda}\tilde{h}}}{\partial\tilde{\beta}}, \tag{12}$$

$$\langle R^2\rangle=-\frac{\partial W_{\tilde{\beta}\tilde{\lambda}\tilde{h}}}{\partial\tilde{\lambda}}, \tag{13}$$

$$\langle P_r(r)\rangle=\frac{1}{\beta r}\frac{\partial W_{\tilde{\beta}\tilde{\lambda}\tilde{h}}}{\partial\tilde{h}}. \tag{14}$$

In heavy ion collisions, the values taken by these state variables are consequences of the dynamics. They cannot be accessed by a statistical treatment but have to be extracted from simulations and/or directly inferred from the data themselves. Equation (11) is exact for an ideal gas. In the case of a strongly interacting system, the underlying hypothesis is that the only relevant information at the freeze-out time is given by the total energy, volume, and collective flow. In the following we take Eq. (11) as an ansatz for the statistical description of an expanding system and explore its properties within a classical system of $N=147$ Lennard-Jones particles of mass m [29]. We expect this ansatz to be reasonable in the case of loose interaction or moderate flows appearing at times close to the freeze-out time, and in the case of a fast reorganization of the potential energy surface, leading to a decoupling of the relaxation time of the interaction and kinetic energy. The adequacy of Eq. (11) to describe the time-dependent expansion of the system will be explored in a forthcoming presentation [35].

The statistical ensemble described by Eq. (11) is similar to a standard Gibbs equilibrium in the local expanding frame, with two important differences with respect to the standard scenario [23,26] of a complete decoupling between collective and thermal motion. First, the energy conservation constraint acts on the total energy, including flow. This allows energy exchanges between the thermal and the collective motions, and therefore can modify considerably the partition's weight, as we show below. Second, Eq. (11) contains a term proportional to r^2 which plays the role of an external pressure [25]. This term is the combination of a positive (out-going) pressure due to the expansion, and a negative pressure term imposing a finite system size at the freeze-out time. This pressure constraint naturally arises from the closed Lie algebra structure of the three operators $\hat{r}^2$, $\hat{p}^2$, and $\hat{\vec{r}}\cdot\hat{\vec{p}}+\hat{\vec{p}}\cdot\hat{\vec{r}}$. If the observables characterizing a system at time t include a collective flow $\langle\hat{\vec{r}}\cdot\hat{\vec{p}}\rangle$, the formalism developed in Sec. II allows this flow observation to be associated with a former time when flow was absent, and the distribution was constrained by the $\langle\hat{r}^2\rangle$ constraint. In turn, this implies that the correct ensemble for treating an open flowing system is not the usual (N,V,T) or (N,V,E) ensemble [23,26,36] but rather an "isobar" ensemble, where the system square radius is constrained only on average through a Lagrange parameter. This is an important point, since it is well known that different statistical ensembles are not equivalent in finite systems [37,38]. In particular, only in such an isobar ensemble is the heat capacity expected to be negative [36] at the liquid-gas phase transition [37], which is at the origin of intense research in the nuclear multifragmentation field [39]. It is generally assumed by statistical models that fragment or hadron partitions are set within a characteristic volume (freeze-out volume) which may depend on the thermal energy, but does not depend on flow [23,26,40,41]. In this case, the presence of flow does not affect the canonical configuration space of the isobar ensemble. Then flow can modify the partitions only because of the modified particle correlations in phase space [12,20,22,42], and because the microcanonical constraint acting on the total energy leads to a nontrivial coupling between thermal and collective energy [20].

III. SYSTEMS IN A HARMONIC TRAP

It is interesting to notice that Eq. (11) is formally identical to a standard Gibbs equilibrium with an external harmonic potential $\hat{U}=\tilde{\lambda}/\tilde{\beta}\Sigma_i\hat{r}_i^2$. The deep connection between an $\hat{R}^2$ constraint and radial collective motion is shown by the fact that it is extremely difficult from a technical point of view to equilibrate a Lennard-Jones system in a harmonic trap; this situation is referred to in the literature as "the harmonic oscillator pathology" [43,44].

A. Dynamics of Lennard-Jones systems

The system under study is composed of $N=147$ particles interacting via a Lennard-Jones (LJ) 6-12 potential with a cutoff radius $r_c=3\sigma$. Energies are measured in units of the potential well (ε), σ characterizes the radius of a particle,

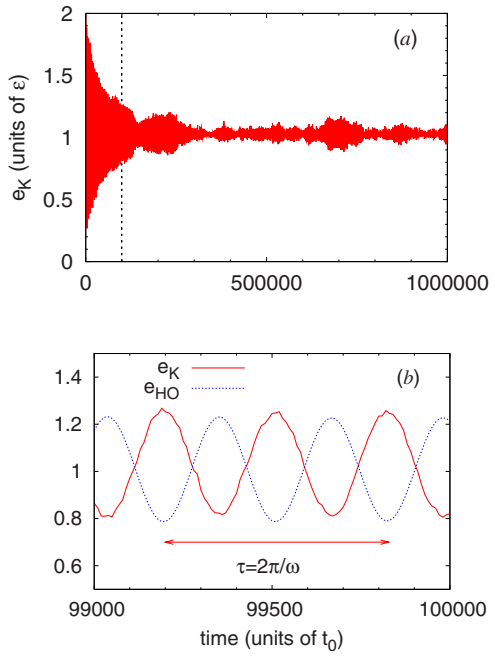

FIG. 1. (Color online) (a) Total kinetic energy per particle as a function of time (in Lennard-Jones units) for a Lennard-Jones system of 147 particles trapped in a harmonic oscillator of spring constant k such that $\omega=\sqrt{k/m}=0.01t_0^{-1}$ for a total energy per particle $e=2.0\varepsilon$. (b) Zoom of the oscillation dynamics over a reduced time interval. Dashed line: potential energy associated with the collective oscillation $e_{HO}=\langle k\hat{r}^2/2\rangle$.

and m is its mass. We adopt adimensional "Lennard-Jones" units for energy, length, and time such that $\epsilon=\sigma=1$, $t_0=\sqrt{\sigma^2 m/48\varepsilon}$ [45]. Initial conditions are constructed from dense drops by rescaling velocities according to a Maxwellian distribution such that the system has the desired value of energy [29–32].

The set of classical equations of motion are integrated using the well-known velocity Verlet algorithm which preserves volume in phase space [43], taking $t_{int}=0.01t_0$ as the integration time step such that the total energy and angular momentum are conserved to better than 0.01% [29,32]. The center-of-mass momentum conservation is better than 1/10 000.

Figure 1 shows a single, very long molecular dynamics run for the Lennard-Jones particles trapped in a harmonic oscillator.

Even if the amplitude of the initial oscillations is damped by the interparticle interaction, it is apparent from Fig. 1 that collective oscillations persist over extremely long times and the ergodic limit does not seem to be attained. This situation is virtually independent of the oscillator frequency and total energy, as well as of the chosen initial conditions for the simulation.

A similar behavior was predicted in Ref. [1] for a system of noninteracting particles. For the sake of clarity, the formalism introduced in Ref. [1] is here briefly recalled. Let us consider as above an initial condition given by Eq. (1) within the ideal gas $\hat{H}=\hat{E}_K+k\hat{R}^2/2$ or diluted Boltzmann limit. If the only constraint on the size is given by the harmonic potential, the density matrix Eq. (1) is a stationary solution of the Liouville equation. If, conversely, the system is initialized to a different average size through an extra constraint $\lambda_0\neq 0$, the system will evolve with the appearance of a collective flow $\hat{B}^{(1)}=-\Sigma_n\frac{1}{m}(\hat{\vec{p}}_n\cdot\hat{\vec{r}}_n+\hat{\vec{r}}_n\cdot\hat{\vec{p}}_n)$ as in Eq. (6). Contrary to the case of a freely expanding system, the successive constraining operators $\hat{B}^{(p)}$ do not vanish for any $p\geq 1$ and can be written as

$$\hat{B}^{(2p)}=\sum_{i=1}^{N}(-1)^p(2\omega)^{2p}\left(\frac{\hat{r}_i^2}{2}-\frac{\hat{p}_i^2}{2mk}\right), \tag{15}$$

$$\hat{B}^{(2p+1)}=-\sum_{i=1}^{N}(-1)^p(2\omega)^{2p}\frac{\hat{\vec{p}}_i\cdot\hat{\vec{r}}_i+\hat{\vec{r}}_i\cdot\hat{\vec{p}}_i}{m}, \tag{16}$$

with $\omega=\sqrt{k/m}$. This gives at any time a density matrix with the same functional form as Eq. (8), with an effective temperature $\tilde{\beta}$, constraining field $\tilde{\lambda}$, and collective radial velocity $\tilde{\nu}$ oscillating in time.

For the purpose of getting analytical results it is easier to consider an initial condition in the canonical ensemble

$$\hat{D}_{\beta_0,\lambda_0}(t_0)=\frac{1}{Z_{\beta_0,\lambda_0}}\exp(-\beta_0\hat{H}-\lambda_0\hat{R}^2). \tag{17}$$

The series Eq. (3) can be analytically summed up, and the time-dependent partition sum $Z_{\tilde{\beta},\tilde{\lambda},\tilde{\nu}}=z^N_{\tilde{\beta},\tilde{\lambda},\tilde{\nu}}$ results, with

$$z_{\tilde{\beta},\tilde{\lambda},\tilde{\nu}}(t)=\mathrm{Tr}\left[\exp\left(-\tilde{\beta}(t)\frac{\hat{p}^2}{2m}-\tilde{\lambda}(t)\hat{r}^2+\frac{\tilde{\nu}(t)}{2}(\hat{\vec{p}}\cdot\hat{\vec{r}}+\hat{\vec{r}}\cdot\hat{\vec{p}})\right)\right]. \tag{18}$$

The time-dependent Lagrange parameters are given by

$$\tilde{\beta}(t)=\beta_0-\frac{\lambda_0}{k}(\cos 2\omega\Delta t-1), \tag{19}$$

$$\tilde{\lambda}(t)=\frac{1}{2}[\beta_0 k+\lambda_0(\cos 2\omega\Delta t+1)], \tag{20}$$

$$\tilde{\nu}(t)=\frac{\lambda_0}{m\omega}\sin 2\omega\Delta t. \tag{21}$$

Equation (18) can be interpreted as a standard Gibbs equilibrium in the rest frame of a breathing system. For classical particles, the trace over single-particle microstates is a phase-space integral $\mathrm{Tr}(\,)=(2\pi\hbar)^{-3}\int d^3r\int d^3p$, where the integrals are evaluated over the whole phase space. The canonical partition sum is readily evaluated:

$$z_{\tilde{\beta},\tilde{\lambda},\tilde{\nu}}(t)=\sqrt{2}m[2\pi\hbar^2(2\tilde{\beta}\tilde{\lambda}-\tilde{\nu}^2 m)]^{-3/2}. \tag{22}$$

This leads to the prediction for the time-dependent behavior of the different observables

$$\frac{\langle p^2\rangle}{2m}=-\frac{\partial\ln z_{\tilde{\beta}\tilde{\lambda}\tilde{\nu}}}{\partial\tilde{\beta}}=\frac{3\tilde{\lambda}}{2\tilde{\beta}\tilde{\lambda}-\tilde{\nu}^2 m}, \tag{23}$$

$$\langle r^2 \rangle = -\frac{\partial \ln z_{\tilde{\beta}\tilde{\lambda}\tilde{\nu}}}{\partial \tilde{\lambda}} = \frac{3\tilde{\beta}}{2\tilde{\beta}\tilde{\lambda} - \tilde{\nu}^2 m}, \tag{24}$$

$$\langle \vec{p} \cdot \vec{r} \rangle = \frac{\partial \ln z_{\tilde{\beta}\tilde{\lambda}\tilde{\nu}}}{\partial \tilde{\nu}} = \frac{3m\tilde{\nu}}{2\tilde{\beta}\tilde{\lambda} - \tilde{\nu}^2 m}. \tag{25}$$

Introducing the expressions for $\tilde{\beta}, \tilde{\lambda}, \tilde{\nu}$, we get

$$e_K \equiv \frac{\langle p^2 \rangle}{2m} = \frac{3}{2\beta_0} \frac{1 + x(1 + \cos 2\omega \Delta t)/2}{1 + x}, \tag{26}$$

$$e_{HO} \equiv \frac{k}{2} \langle r^2 \rangle = \frac{3}{2\beta_0} \frac{1 + x(1 - \cos 2\omega \Delta t)/2}{1 + x}, \tag{27}$$

$$e_{flow} \equiv \omega \langle \vec{p} \cdot \vec{r} \rangle = \frac{3}{2\beta_0} \frac{x}{1 + x} \sin 2\omega \Delta t, \tag{28}$$

where the initial constraint λ_0 has been rewritten such that $x = 2\lambda_0 / k\beta_0$ measures its strength. It is clear from the inspection of Fig. 1 that over the time scale of a collective oscillation the interparticle interaction can be neglected, the total energy conservation constraint does not seem to play an important role, and the canonical free-particle result Eq. (18) appears fairly accurate. The kinetic energy does oscillate with twice the oscillator frequency in phase opposition, this collective motion breaking the ergodicity of the dynamics. We observe this same ideal gas behavior for several oscillator frequencies between $0.001 t_0^{-1}$ and $0.2 t_0^{-1}$, and energies between -1.0ε and 2.0ε.

B. Microcanonical thermodynamics

In order to study the effect of flow for the freely expanding system, we have performed numerical molecular dynamics calculations within the statistical ensemble Eq. (11) without $(h=0)$ and with $(h>0)$ the contribution of a radial collective flow. To study the thermodynamical properties of the isobar ensemble characterized by a size constraint λ_0, we have constructed the microcanonical distribution by sorting the events as a function of the energy for a canonical ensemble [46] of the equivalent system trapped in a harmonic oscillator of spring constant $k = 2\lambda_0 / \beta$. The canonical distributions are obtained by coupling the system to a thermostat with the Andersen technique [47]. In brief, the coupling is made by stochastic impulsive forces that act occasionally on randomly selected particles. After each collision, the selected particle is endowed with a new velocity drawn from a Maxwell-Boltzmann distribution at the desired canonical temperature. The combination of Newtonian dynamics with the stochastic collisions generates a Markov chain in phase space, which under some general conditions generates the canonical distribution [47].

The resulting microcanonical temperature and kinetic energy fluctuations are shown in Fig. 2 for an oscillator frequency $\omega = 0.01 t_0^{-1}$. Close to the liquid-gas transition temperature, the canonical calculations give rise to very wide energy distributions and the different events (n) can be sorted in total energy bins

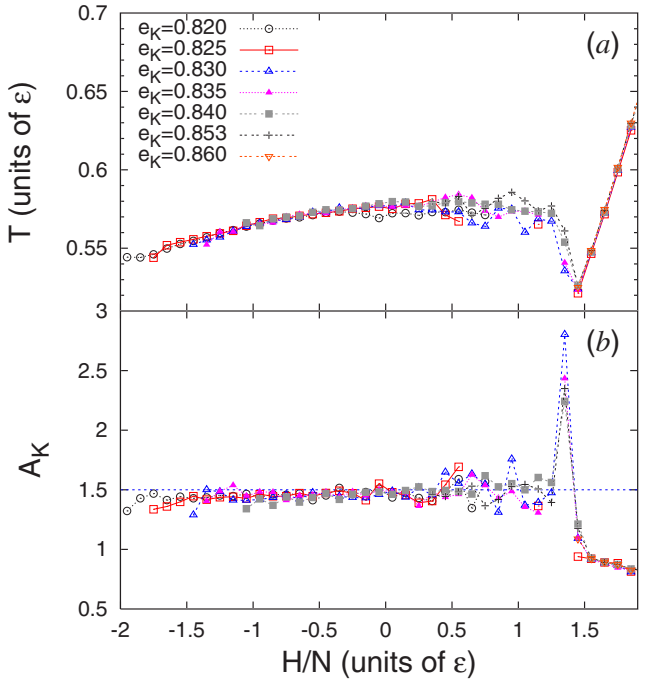

FIG. 2. (Color online) Microcanonical temperature (a) and normalized kinetic energy fluctuation (b) as a function of the total energy inside the harmonic oscillator obtained from an energy sorting of the canonical distributions corresponding to an oscillator frequency $\omega = 0.01 t_0^{-1}$, and canonical temperatures $\beta = 3/(2e_K)$ as indicated. All quantities are expressed in Lennard-Jones units.

$$H_n = E_{Kn} + E_{LJn} + \frac{1}{2} k R_n^2. \tag{29}$$

This energy can be physically interpreted as a free enthalpy for the isolated unbound system characterized by a finite size at the freeze-out time [46]. Each single canonical sampling, for which the inverse of the canonical temperature β^{-1} is controlled, can therefore be used to access the microcanonical thermodynamics over a wide enthalpy region. The microcanonical temperature is evaluated in each enthalpy bin as $T(H) = 2\langle e_K \rangle / 3$ [37], where the average is taken over events belonging to the same bin. The normalized kinetic energy fluctuation $A_K = N(\langle e_K^2 \rangle - \langle e_K \rangle^2)/T^2$ is also represented. The nice agreement between estimations obtained with different canonical temperatures shows the quality of the numerical sampling. Figure 3 shows the dependence of the results on the oscillator strength. We can recognize for low ω values, i.e., loose constraints on the system size, the first-order liquid-gas phase transition. The transition is signaled by the back bending of the microcanonical caloric curve [36], corresponding to a negative heat capacity, and the associated abnormal kinetic energy fluctuation overcoming the canonical limit $A_K = 3/2$ [37]. The consistency between the two independent signals is again a proof of the numerical quality of the microcanonical sampling. These results are in qualitative agreement with the ones obtained for the lattice gas model in the same ensemble [46]. Interestingly, in the energy interval corresponding to the transition, the mean square radius shows a kink and a slope change at higher energies. The spatial extension of the unbound phase grows

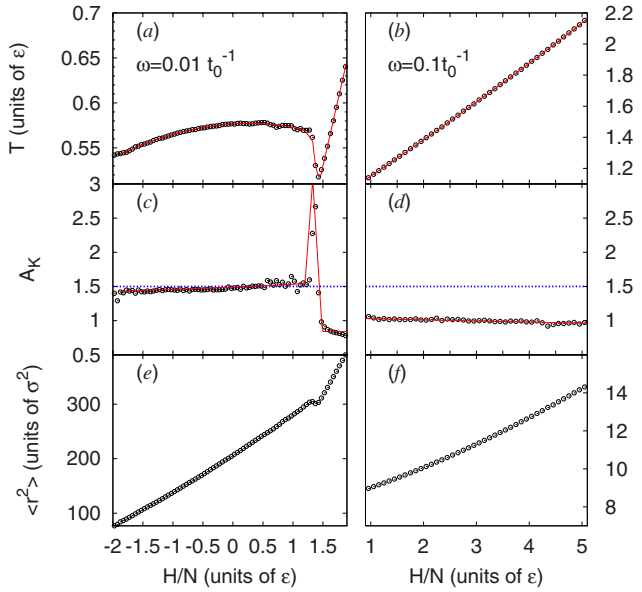

FIG. 3. (Color online) Microcanonical temperature (a),(b), normalized kinetic energy fluctuation (c),(d), and mean square radius (e),(f) as functions of the total energy inside the harmonic oscillator for two different oscillator strengths. The horizontal lines in the middle panels give the fluctuation expected in the canonical ensemble.

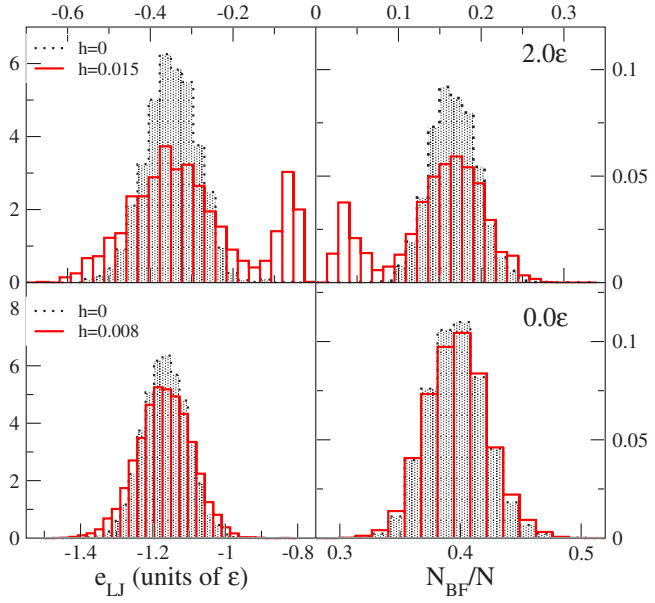

FIG. 4. (Color online) Distributions of potential energy (left side) and of the size of the largest cluster (right side) at two different thermal energies corresponding to the bound phase (lower part) and close to the transition region (upper part). The filled histograms correspond to a static equilibrium $h=0$ while for the empty ones flow was included according to Eq. (11). All quantities are expressed in Lennard-Jones units.

more rapidly with the energy, and at the coexistence point the two phases have similar spatial extensions. This means that in this model, contrary to the lattice case [37], the two coexisting phases at the transition temperature can be populated even in an ensemble that strongly constrains the volume of the system. In particular, the two characteristic signals of a first-order phase transition in a finite system, namely, bimodality in the canonical ensemble and negative heat capacity in the microcanonical one, can be observed even in the isochore ensemble [30,31].

For stronger size constraints (smaller average volumes), the caloric curve is monotonic, the microcanonical constraint reduces fluctuations well below the canonical limit, and the mean square radius increases linearly with the energy. This signals a supercritical system. From these calculations, the critical pressure, at which the back bending of the microcanonical caloric curve disappears, can be roughly estimated as $\omega_c \approx 0.015 t_0^{-1}$.

IV. MICROSTATE DISTRIBUTIONS IN AN EXPANDING ENSEMBLE

To simulate the expanding ensemble Eq. (11), a radial momentum $\vec{p}_r = m\tilde{h}r\vec{u}_r$ is added to each particle and a microcanonical sorting is imposed on the total energy including flow, $E' = \Sigma_i(\vec{p}_i + \vec{p}_{ri})^2/(2m) + E_{LJ}$. The Hubble factor $\tilde{h}$ employed at different energies has been obtained from the measured collective velocity of the same system freely expanding in vacuum (E_{flow}^{free}) according to $h^2/2m\langle R^2\rangle = E_{flow}^{free}$ [32]. Since the addition of flow trivially increases the total energy E, such that $E' = \langle E_{th}\rangle + \langle E_{flow}\rangle > E$, the comparison between the calculations without flow at an energy E and those of the ensemble including flow at an energy E' have to be made such that the average thermal energies of both systems are similar, $\langle E_{th}\rangle = E$.

The results are shown in Fig. 4 for the distribution of the potential energy and the size of the largest fragment recognized through the minimum spanning tree (MST) algorithm [29]. We can see that for all energies the presence of flow modifies the distributions in a sizable way, leading to higher fluctuations. This is easy to understand from Eq. (11) if we consider that in the expansion dynamics only the total energy is conserved, meaning that thermal energy fluctuations can be compensated by collective energy fluctuations. In this sense, the collective motion acts as a heat bath, leading to distributions similar to the canonical ones. In particular, if the system has a total energy inside the coexistence region of the first-order phase transition (upper part of Fig. 4) the exchange with the flow reservoir can allow the system to explore the two coexisting phases. These latter differ in potential energy $\Delta e_{LJ} \approx 0.4\varepsilon$ but not in average spatial extension (see Fig. 3) and can therefore be accessed in the same ensemble for a given value of the average freeze-out volume.

This result implies that signals of phase transitions typical of the canonical ensemble, such as bimodalities, can be pertinent also in the microcanonical framework, if flow is accounted for in a thermodynamically consistent way. Then such signals may be accessed even in experimental situations where the deposited energy is strongly constrained. A possible experimental confirmation of this prediction in nuclear multifragmentation can be found in Ref. [48].

At this point a word of caution is in order. Our ansatz (11) is exact only for a system of noninteracting particles (or in

the limit of local interactions). In the presence of strong correlations this ansatz supposes the system relaxation time to be small compared to the time scale of the expansion. This condition should be satisfied if the average collective velocity $\langle v_F \rangle$ is much smaller than the velocity associated with the thermal motion, $\langle v_{th} \rangle$. Within the ansatz (11), the local equation of state for the radial momentum reads

$$\langle p_r(r) \rangle \approx \frac{1}{r} \frac{\partial \ln z}{\partial(\tilde{\beta}\tilde{h})} = \tilde{h} m r, \tag{30}$$

where we have neglected the effect of the energy-conserving δ function in Eq. (11) in order to have an analytical order-of-magnitude estimate. This leads to a collective velocity $v_F = \tilde{h}\langle R \rangle$, which should be compared to the canonical estimate $v_{th} = \sqrt{3/(\tilde{\beta}m)}$. In the case of the upper part of Fig. 4 we have $v_F / v_{th} \approx 0.79$, meaning that the quality of our approximation may be doubtful. It is, however, interesting to note that the bimodal shape of the distribution in the presence of flow persists also for smaller collective motions, as long as the energy fluctuations are of the order of the energy distance Δe_{LJ} between the two phases.

V. CONCLUSIONS

To conclude, in this paper we have applied an information-theory-based formalism allowing us to include collective motions in the statistical description of finite unbound systems for the flow dynamics of classical Lennard-Jones particles. Molecular dynamics simulations show that the simplifying ideal gas approximation worked out in Ref. [1] may be of some pertinence even for dense, strongly interacting systems: the time behavior of the different energy components closely follows the ideal gas predictions. This behavior can be understood from the closed algebraic structure of the $\hat{p}^2$, $\hat{r}^2$, and $\hat{\vec{r}} \cdot \hat{\vec{p}}$ operators, which completely dominates the dynamics of the expansion. In the ideal gas limit, the flow is self-similar, meaning that the distribution can be recast as an equilibrium in the local rest frame in an effective pressure field. Our simulations demonstrate that even in this approximation of noninteracting particles, the presence of flow can influence the microstate distribution in a sizable way. Indeed, the presence of a (nonconserved in time) collective energy component can play the role of a heat bath, allowing for extra configurational energy fluctuations in the total energy-conserving dynamics. In particular, close to a first-order phase transition, this mechanism is seen to give rise to a characteristic bimodal behavior, similar to some recent experimental observations in nuclear multifragmentation.

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