Equilibrium under flow

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Using information theory we derive a thermodynamics for systems evolving under a collective motion, i.e. under a time-odd constraint. An illustration within the Lattice gas Model is given for two model cases: a collision between two complex particles leading to an incomplete relaxation of the incoming momentum, and a self-similar expansion. A semi-quantitative connection with the determination of thermodynamical quantities in multifragmentation reactions is done showing that they are affected in a sizeable way only when the flow dominates the global energetic.

PACS numbers: 64.10.+h, 25.75.Ld, 25.70.Pq

Heavy ion collisions represent a unique opportunity to probe the interdisciplinary field of phase transitions in mesoscopic systems for which a non standard thermodynamics giving rise to negative heat capacities is predicted [1]. An indication of negative heat capacities has been experimentally found [2] in multifragmentation reactions. These results can be considered as a first step towards a quantitative determination of the nuclear phase diagram. Negative heat capacities have also been observed in simulations of self-gravitating systems [3] and in the melting and boiling of clusters [4].

An important conceptual problem linked with multifragmentation experiments is that the outcomes of a nuclear collision are not confined in an external container but dynamically deexcite in the vacuum. In the absence of boundary conditions, collective flows can be present at the fragmentation time. Because of this time odd component, one may doubt about the applicability of equilibrium concepts. However, we will show that information theory allows a thermodynamically consistent description of open finite systems in evolution under a collective flow. We will apply this formalism to the Lattice Gas Model [5] for the particular cases of a memory of the entrance channel (transparency) and radial expansion. In both cases the properties of the system appear to be affected in a sizeable way when flow dominates the global energetics.

In the Gibbs formulation of statistical mechanics an equilibrium is defined as a collection of different microstates all corresponding to the same macrostate (or statistical ensemble) defined through the average value of (a collection of) collective variables. A practical realization of a Gibbs ensemble is given by the collection of different snapshots of an isolated ergodic system evolving in time, provided that the observation time is much longer than a typical equilibration time. This type of statistical ensemble is not very useful for short-lived open systems as the transient excited states formed in a nuclear collision. However, ergodicity is not the unique way to produce a Gibbs ensemble. Indeed, within information theory, an equilibrium corresponds to any ensemble of states that maximizes the entropy in a given space under the constraint of (a number of) observables known in average [6]. Therefore, if the nuclear dynamics is sufficiently sensitive to the initial conditions, the ensemble of outcomes of similarly prepared nuclear collisions can be considered as a statistical ensemble for which the important observables are controlled by the dynamics (and by the event sorting performed on specific observables). As an example, in the standard freeze out hypothesis the configurations are fixed when the nuclear interaction among prefragments becomes negligible; then the ensemble of events is characterized by several variables such as the energy and the spatial extension $R^2$ which for open systems is fluctuating event by event. This can be accounted for by considering the ensemble average $\langle R^2 \rangle$ as a state variable and introducing a Lagrange multiplier $\lambda$ closely related to a pressure. In this information theory approach, the state variables are determined by the dynamics and can also be time odd quantities such as transparency or radial flow.

Let us first consider a symmetric head-on collision with a too short reaction time to fully relax the incoming momentum. This situation seems to be verified at relativistic energies [2]. It corresponds to the observation of an additional one body state variable, the memory of the initial momenta $\langle \epsilon p_z \rangle$, where $p_z$ is the momentum along the beam axis and $\epsilon = -1(+1)$ for the particles initially belonging to the target (projectile). Let us assume that the total energy $E$ is also known only in average. The maximization of the entropy leads to the partition sum of the incomplete momentum relaxation ensemble (IMRE)

$$Z_{\beta, \alpha} = \sum_n \exp \left( -\beta E^{(n)} + \alpha \sum_{i=1}^{A} \epsilon_i p^{(n)}_z \right)$$

(1)

where the indice $i$ stands for the $i$-th particle while $n$ counts the events. $\beta$ and $\alpha$ are Lagrange multipliers associated to the constraint of the degree of incomplete stopping $\langle \epsilon p_z \rangle$ and of the total center of mass energy $< E >$. The relative probability of an event $n$ results

$$p^{(n)} \propto \exp \left[ -\beta \left( \sum_{i=1}^{A} \frac{\left( p^{(n)}_i + \epsilon_i \overline{p}_0 \right)^2}{2m} + \sum_{ij} U_{ij} \right) \right]$$

(2)

where $U_{ij}$ is the two body interaction and we have introduced $\overline{p}_0 = m\alpha/\beta u_z^0$. The average kinetic energy is
velocity 2
interpreted as two thermalized sources with a non zero relative

\[ \lambda_R \]
fluctuation, while a term

\[ \delta p \]
along the beam axis \( \vec{u}_z \). In actual heavy

\[ p_0 = 0 \], these expressions correspond to the usual canoni-
cal ensemble while in the general case they can be inter-

\[ \lambda \]
leads to

\[ p = 0 \]
states related to

\[ \lambda \]
\( n \) = 216 particles at a subcritical pressure

\[ \beta = 0.65 \epsilon \] which cor-
responds to the transition temperature in the canonical

\[ \Delta p / p = \frac{\sqrt{2} < |p_z| > - < |p_\perp| >}{2(\sqrt{2} < |p_z| > + < |p_\perp| >)} \]
(3)
A quantitative comparison with experimental data would
require to fix the Lagrange parameters \( \lambda, \beta, p_0 \) from each
specific set of data and to include quantum effects and
symmetry as well as Coulomb terms in the hamiltonian,
however from this illustrative example we can clearly see
that partitions are affected by a collective longitudinal
component and a higher degree of fragmentation does
not necessarily imply higher temperatures but can also
be consistent with an increased degree of transparency
of the collision. To quantify this statement, Figure 1b
compares the clusters size distributions of the IMRE at a
fixed total energy with the standard microcanonical en-
samble (fixed energy, spherical momentum distribution)
at the same energy. It is clear that thermal agitation
is much more effective than transparency to break up
the system: at the energy where the microcanonical en-
samble predicts a complete vaporization of the system,
a residue persists if the non relaxed momentum compo-
nent is as large as the relaxed one. This is in qualita-
tive agreement with the trend observed in central colli-
sions at relativistic energies \[ \lambda \]. On the other side up
to 10% transparency the distributions are almost identi-
cal, meaning that when the velocity difference between
the quasi-projectile and the quasi-target is of this order,
the debate on equilibrium based on the number of emis-

\[ < E_k > /A = 3/(2\beta) + p_0^2/(2m) \] while the equation of
states related to \( \alpha \) leads to

\[ < cp_z > = A p_0 \]. In the limit

\[ p_0 = 0 \], these expressions correspond to the usual canoni-
cal ensemble while in the general case they can be inter-

\[ \lambda \]
leads to

\[ p = 0 \]
states related to

\[ \lambda \]
\( n \) = 216 particles at a subcritical pressure \( \lambda = 3.3 \cdot 10^{-4} \)
and clusters are defined within the standard Coniglio-

Klein prescription\[ \lambda \]. Since in this classical approach
the configurational and kinetic partition sums are fac-
torized, for a given \( \beta \) the lattice configurations will be
independent of the degree of transparency \( p_0 \). However
the active bond probability will explicitly depend on \( p_0 \)
meaning that cluster observables can be affected by the
incomplete relaxation. Figure 1a shows the cluster size

\[ \delta |p_z|^2 \]
control the collective flow fluctuation, while a term

\[ \lambda |H(n)|^2 \] can be used to impose an average freeze out volume. For simplicity in the follow-

\[ \beta /2m + \delta \]
the longitudinal momentum dispersion has been kept fixed,

\[ (\beta /2m + \delta)^{-1} = 0.04 \epsilon \].

To understand the effect of transparency on the eval-
uation of thermodynamical quantities we have used the
Lattice Gas hamiltonian \[ \lambda \] where occupied sites on a
three dimensional cubic lattice interact via a constant
closest neighbors coupling \( \epsilon \). This simple but numeri-
cally solvable model is isomorphous to the Ising model
in the grancanonical ensemble and constitutes therefore
a paradigm of standard equilibrium statistical mechanics
with first and second order phase transitions. Calcula-
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sion sources \[14\] is an academic question. The important influence of the collective component on the cluster distributions means that, if the incoming momentum is not completely relaxed, the methods used to determine thermodynamical quantities can be strongly biased. Indeed if energy is divided into a kinetic \(e_k\) and an interaction \(e_i\) component, the average kinetic energy can be used as a microcanonical thermometer while the normalized partial energy fluctuations are linked to the microcanonical heat capacity \[3\]. The interaction energy can be estimated as the Q-value of the detected fragments \[2\]. Figure 2 shows the deformation induced by transparency on the first and second order moments of partial energies that are used to infer the temperature and heat capacity in the microcanonical sorting of fragmentation data \[3\]. The Q-value can be computed in the Lattice Gas model in a liquid drop approximation as

\[
Q^{(n)} = \sum_{i=1}^{M^{(n)}} a_v A_i + a_s A_i^{2/3}
\]

where \(M^{(n)}\) is the multiplicity of the n-th event and \(a_v, a_s\) are the volume and surface energy coefficients. The average kinetic energy and the average Q-value obtained with eq.\[4\] are shown in the left part of figure 2 for the microcanonical ensemble and for a system with the same total deposited energy and an increasing degree of transparency \(\Delta p/p\). The energy range explored corresponds to the phase transition region. The increased probability of heavy clusters with an increasing degree of transparency shown in figure 1 induces an overestimation of the average kinetic energy, hence of the estimated temperature. The peak in the partial energy fluctuation which signals the phase transition \[8\] disappears in this extreme scenario of an increase of energy going entirely into the relative motion of the two sources, and the normalized fluctuations are systematically lower than in the microcanonical ensemble where the incoming momentum is fully relaxed. Since a negative heat capacity corresponds to abnormally high partial energy fluctuations \[8\]. Figure 2 implies that an incomplete relaxation of the incoming momentum can prevent the observation of negative heat capacity.

Another important form of collective motion in heavy ion collisions is radial flow which starts to be observed in central collisions around 30 A MeV incident energy \[14\] and becomes the dominant fraction of the detected energy in the relativistic domain \[13\]. We can describe this dynamical situation in the framework of information theory as an equilibrium with non random directions for velocities which are preferentially oriented in the radial direction. In the canonical formulation this corresponds to two independent observations of the average energy \(<E>_0\) and a the average local radial momentum \(<p_r>_0\). The probability of a microstate \((n)\) reads

\[
p^{(n)} \propto \exp \left( -\beta E^{(n)} - \sum_{i=1}^{A} \gamma(r_i) \mathbf{p}_i \cdot \mathbf{u}_{r_i} \right)
\]

where \(r_i\) is the center of mass position of the i-th particle and \(\beta, \gamma(r)\) are Lagrange multipliers. Imposing in the local equation of state \(<p_r)_0 = \partial \log Z/\partial \gamma\) that the observed velocity is self-similar \(<p_r>_0 = m \alpha r_0 \) we obtain \(\gamma(r) = -\beta \alpha r\) which gives for the argument of the exponential in the probability \[6\]

\[
\frac{-\beta}{2m} \left( \mathbf{p}_i - \mathbf{p}_0(r_i) \right)^2 + \frac{\beta \alpha^2 m}{2} \sum_{i=1}^{A} r_i^2 - \beta E_{pot}
\]

with the local radial momentum \(\mathbf{p}_0(r_i) = m \alpha r_0 \). The situation is equivalent to a standard Gibbs equilibrium in the local expanding frame. This scenario is often invoked in the literature \[14\] to justify the treatment of flow as a collective radial velocity superimposed on thermal motion; however eq.\[6\] contains also an additional term \(\propto r^2\) which corresponds to an outgoing pressure. This term cannot be avoided in the selfsimilar scenario; indeed the total average energy under flow reads \(<E>_0 = 3/(2\beta) + <E_{pot} > + ma^2/2 <R^2>_0\) where we have used the fact that the scalar product between the flow and the thermal component is in average zero. The probability under flow eq.\[6\] diverges at infinity reflecting the trivial dynamical fact that asymptotically particles flow away. This divergence should be cured by introducing an external confining pressure which is not a mathematical artifact but has to be interpreted as discussed above as a Lagrange multiplier imposing a finite freeze out volume. Eq.\[6\] has then to be augmented by a term \(-\lambda \sum_i r_i^2\) with \(\lambda \geq ma^2/2T\) leading to a positive

![FIG. 3: Upper left: effective pressure (full line) and average volume (dashed line) as a function of the collective radial velocity. Upper right and lower part: fragment size distributions in the expanding Lattice Gas model. Distributions without flow (full black lines) are compared with distributions with 10% (dashed black), 30% (full grey) and 60% (dashed grey) contribution of radial flow at the same temperature (upper right) and at the same total energy (low part). Symbols: calculations with flow at the same thermal energy and average volume as the full black lines.](image-url)
The effective pressure $\lambda_{eff}$ as well as the associated average volume (normalized to the ground state volume $V_0 = A$) are shown in the upper left part of figure 3 as a function of the collective radial velocity for a given pressure $\lambda = 1.23 \cdot 10^{-2}$ and temperature $\beta^{-1} = 0.65 \varepsilon$. The Lagrange parameter $\lambda_{eff}$ being a decreasing function of $\alpha$, the flow reduces the effective pressure so that the critical point is moved towards higher pressures in the presence of flow [7]. However one can see that the effect is very small up to $ma \approx 0.6$ (which corresponds to $\approx 40\%$ contribution of flow to the kinetic energy). In this regime the cluster size distributions displayed in the upper right part of figure 3 are only slightly affected. On the other side if the collective flow overcomes a threshold value $\Delta E_k/E_k \approx 50\%$ the average volume (dashed line in fig.3a) shows an exponential increase and the outgoing flow pressure leads to a complete fragmentation of the system (dashed grey line in fig.3b). Again an oriented motion is systematically less effective than a random one to break up the system. This is shown in the lower part of figure 3 which compares for a given $\lambda$ distributions with and without radial flow at the same total deposited energy: for any value of radial flow equilibrium in the system (dashed grey line in fig.3b). Again an oriented motion is systematically less effective than a random one to break up the system. A consequence of that is that normalized partial energy fluctuations for partially fragmented configurations. Concerning heavy ion collisions, it is important to stress that the pressure $\lambda$ as well as the other 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 data itself [2]. Different models assume that fragmentation occurs in an average freeze out volume which may depend on the thermal energy but does not depend on flow. This is true if the system fragments at the turning point of its expansion ($\lambda_{eff} = 0$) [14] or when the interaction between fragment surfaces becomes negligible [10] or more generally insufficient to modify the N-body correlations [11]. In this case the presence of flow does not affect the configuration space and can only modify the partitions because of the modified microscopic bonds among particles taken into account by the Coniglio-Klein algorithm. However this effect is negligible as already observed by Das Gupta et al. [14] and shown in the lower part of Figure 3. In this figure the symbols represent the size distributions with collective flow at the same thermal energy and average volume as the standard microcanonical results (full lines). Even for the largest amount of flow considered the two distributions are identical, meaning that in this hypothesis all thermodynamical analysis of fragmentation data stay valid in the presence of even strong collective flows [10].

In this paper we have shown that information theory [9] allows to take into account generic collective motions in a rigorous statistical way leading to the formulation of a consistent ”out of (static) equilibrium” thermodynamics. We have particularized this general statement to two kinds of collective motion which are particularly relevant in nuclear multifragmentation, namely partial transparency and radial selfsimilar flow. We have applied the formalism to the Lattice Gas model which has already shown some pertinence [16] to the multifragmentation phenomenology. We have shown that the disordered thermal motion is always more efficient than the collective motion to break up the system. A consequence of that is that normalized partial energy fluctuations for a system under flow are always reduced respect to the standard microcanonical expectation [16] and the negative heat capacity signal experimentally observed [2] cannot be due to the possible presence of a collective component neglected in the data analysis. Transparency leaves the configurational energy unmodified, while radial flow, because of the coupling between r and p space, is shown to be equivalent to an external pressure leading to an increased value of the critical point [7]. Concerning the extraction of thermodynamical variables from fragmentation data, radial flow can be simply subtracted from the detected energy [10] while transparency can be neglected only if the relaxation of the incoming momentum exceeds about 90\%.

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