THERMODYNAMICS OF EXPLOSIONS

G. NEERGAARD
Niels Bohr Institute, Blegdamsvej 17, DK - 2100 Copenhagen, Denmark
Institute of Physics and Astronomy, University of Aarhus, DK - 8000 Aarhus
E-mail: neergard@nbi.dk

J. P. BONDORF
Niels Bohr Institute, Blegdamsvej 17, DK - 2100 Copenhagen, Denmark
E-mail: bondorf@nbi.dk

I. N. MISHUSTIN
Frankfurt University, D-60054, Germany
and
The Kurchatov Institute, Russian Research Center, 123182 Moscow, Russia
E-mail: mishustin@nbi.dk

We present our first attempts to formulate a thermodynamics-like description of explosions. The motivation is partly a fundamental interest in non-equilibrium statistical physics, partly the resemblance of an explosion to the late stages of a heavy-ion collision. We perform numerical simulations on a microscopic model of interacting billiard-ball like particles, and we analyse the results of such simulations trying to identify collective variables describing the degree of equilibrium during the explosion.

1 Introduction

The assumption of thermodynamic equilibrium at an intermediate stage of a heavy-ion collision is often incorporated in models of the colliding nuclear matter. These models range from statistical models of nuclear multifragmentation to the fluid dynamical models of the quark gluon plasma. In contrast, microscopic models of molecular dynamics type (e.g. RQMD, FMD and NMD), which are based upon constituent interactions, do not contain this assumption. Such models are appropriate for testing to what extent thermodynamic equilibrium is actually achieved. And if it is not, the application of thermodynamic concepts such as temperature and entropy becomes questionable. In this study we employ a very simple model, and focus on the thermodynamic or “overall” description of the system.


2 The model

Our model consists of a number \( A \) of identical balls of radius \( r_{hc} \) having mass \( m \). They perform classical non-relativistic hard-sphere scatterings, conserving energy, momentum and angular momentum. Initially the \( A \) balls are placed randomly within a sphere of radius \( R = R_0 A^{1/3} \), and the initial velocities are chosen as a superposition of thermal (Maxwell-Boltzmann) and collective motion. We use a spherically symmetric Hubble-like flow field for the initial collective motion:

\[
\vec{v}(\vec{r}) = -v_{0f} \frac{\vec{r}}{R}
\]

where \( v_{0f} \) is a model parameter, \( v_{0f} > 0 \) for ingoing flow and \( v_{0f} < 0 \) for outgoing flow. We fix the total energy \( E = E_{fl} + E_{th} \), and vary the fraction \( \eta \) of the flow energy, \( \eta = E_{fl}/E \), where \( E_{fl} = \frac{mv_{0f}^2}{2R^2} \sum_{i=1}^{A} \vec{r}_i^2 \) and \( E_{th} \) are the flow energy and the thermal energy, respectively. Because of the way in which the system is built up, these energies will fluctuate from event to event with a relative uncertainty of the order of \( A^{-2} \).

In our simulations we have chosen nuclear-scale parameters: \( m = 940 \text{ MeV}, r_{hc} = 0.5 \text{ fm}, R_0 = 1.2 \text{ fm}, 0 \leq v_{0f} \leq 0.5 \) (in units of the velocity of light, \( c = 1 \)), but since the behavior of the model only depends on the two combined parameters \( mv_{0f}^2 \) and \( r_{hc}/R \), the choice of nuclear scale is not crucial. We choose \( A = 50 \), so with these parameters the initial radius of the system is 4.2 fm.

We focus on four different types of event: • 'th20': The particles are started in 100\% thermal motion inside a spherical container of radius 4.2 fm, at \( t = 20 \text{ fm/c} \) the container walls are removed. • 'in': 100\% ingoing flow. After interacting, the particles will move out again. This implosion-explosion process is intended to simulate some features of a heavy-ion collision. • '50/50': 50\% thermal motion + 50\% outgoing flow, simulating an explosion from a non-thermalized state. • '100out7': 100\% outgoing flow inside a spherical container of radius 7 fm.

The results are averaged over an ensemble of 20 events of each kind.

3 Thermodynamic considerations

It is clear that we cannot use ordinary thermodynamics (or its well-known extensions to small systems or to small deviations from equilibrium) for the description of the overall behavior of our model. First, it is not clear that equilibrium prevails, even locally. Indeed we wish to investigate to what extent equilibrium is reached in the course of an implosion-explosion process.

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Second, our system has no fixed volume, it expands freely into the vacuum. It is the combination of these two facts, no temperature and no volume, that makes our approach different from much previous work on the subject.

Equilibrium thermodynamics is linked to the motion of the individual constituents making up the macroscopic system via the entropy. A natural starting point for the investigation of the overall, i.e. the “thermodynamic”, behavior of our system is therefore to apply an expression similar to the entropy, but in a way that makes sense in this highly non-equilibrium system.

To study one-body observables, we reduce the $6A$ dimensional phase-space of the $A$ particles to 6 dimensions in the standard way. Then we introduce a finite grid in the reduced phase-space, dividing each of the 6 axes into $D$ segments. Instead of working with a fixed grid in phase-space, which would give us the usual entropy, we let the entire grid expand or contract along with the swarm of points in phase-space in a uniform way: The outer grid edge follows the outermost point, the boxes are of equal size, and the number of boxes is kept fixed, thus the physical size (e.g. in units of $\hbar^3$) of each box in phase-space varies with time. This is to deal with the no volume problem, we mentioned above. We then introduce the pseudo-entropy as

$$\Sigma = -\frac{1}{\xi} \sum_i p_i \log(p_i)$$

where

$$p_i = \frac{\text{number of points in box } i}{\text{total number of points in phase space}}$$

and $\xi$ is a normalization constant. We choose $\xi$ as the theoretical maximum value of $-\sum_i p_i \log(p_i)$ so that $\Sigma \in [0, 1]$. In the current set-up, for the case of $N$ points in a reduced phase-space divided into $D^6$ boxes, $\xi$ is the smaller number of $\log(N)$ and $6 \log(D)$. We refer to the quantity $\Sigma$ as the pseudo-entropy instead of entropy, since some important features of the entropy, e.g. that it increases, are not retained in this formulation. Nevertheless, we shall see that $\Sigma$ has some nice properties, including that of characterizing the degree of equilibrium. For a system of fixed volume in equilibrium, $\Sigma$ is the usual one-body entropy (apart from normalization).

4 Results

In the calculations presented here, we have chosen $D = 7$, so the 6 dimensional phase-space is divided into $7^6$ boxes. Because we are dealing with a small

\[ a \text{ in the limit } D \to \infty \text{ in an ensemble of infinitely many events} \]
number of events (typically 20) in the ensembles, the precise values of $\Sigma$ depend on the choice of grid. We have, however, verified that $\Sigma$ behaves qualitatively similar to what is shown here over a range of grid-sizes, varying $D$ between 2 and 9.

To give an idea of the dynamics and the timescales, we show in Fig. 1 the scattering rate.

**Figure 1.** The scattering rate (number of scatterings per particle per time unit) for the four cases mentioned in the text. In the implosion-explosion event ('in') practically all particles scatter around the time $t \approx 6$ fm/c. This is the time when the system is maximally compressed. Then, as the expansion begins, the scattering rate decreases until $t \approx 15$ fm/c, when interactions have essentially ceased. In the '100out7' case the particles start to hit the container wall at $t \approx 5$ fm/c (the scatterings against the container walls are not counted here), and the peak in the scattering rate at $t \approx 20$ fm/c results from particles moving back after hitting the wall and scattering against other particles still on their way out.

Fig. 2 shows how the pseudo-entropy behaves in each of the four cases. In the 'th20' case, the pseudo-entropy $\Sigma \approx 1$ as long as the particles are in equilibrium at fixed volume inside the container. Then at $t = 20$ fm/c, when the container is removed and the system starts to expand, the pseudo-entropy decreases, reflecting the fact that the system goes out of equilibrium.\(^b\)

In the case '100out7', where the particles are started in an extreme non-equilibrium situation, the pseudo-entropy is low ($\Sigma = 0.8$ is a low value in this context), but increases towards $\Sigma = 1$ as the scatterings equilibrize the system. By comparison with Fig. 1 one can see that the first jump in $\Sigma$ at

\(^b\) The particles stay almost *thermalized*, though, in the sense that they retain their Maxwell-Boltzmann velocity distribution. But they are certainly not in *equilibrium*, since this means that the phase-space distribution is independent of time.
Figure 2. The pseudo-entropy for the four cases described in the text. This variable seems to quantify the degree of equilibrium in the system, $\Sigma = 1$ characterising an equilibrium state.

$t \simeq 5$ fm/c is due to particles scattering against the container wall (when particles hit the wall their velocity is reversed, so in this process many new states in phase-space are being populated), and the second “jump” around $t \simeq 20$ fm/c is due to the many particle-particle scatterings around this time.

The interesting case is the implosion-explosion (‘in’) scenario, since here we do not know in advance if the system reaches a state of equilibrium or not. From the fact that the pseudo-entropy in Fig. 2 reaches a value $\Sigma \simeq 1$, the same value as the known equilibrium case ‘th20’, we infer that the system is in a state of equilibrium around $t \simeq 6$ fm/c (which is also the time of maximum compression). We have checked that the speed distribution of the particles becomes nearly Maxwellian from $t \simeq 6$ fm/c with a temperature in the compressed state of 47 MeV, which is also the theoretical value of the temperature assuming that all of the initial flow energy is converted to thermal energy.

Another interesting feature of the pseudo-entropy is that it seems to decay in a characteristic fashion when the system expands from a state of equilibrium, see Fig. 3.

5 Conclusions

In this note we address the problem of thermodynamic equilibration in the context of heavy-ion collisions. We have defined a variable inspired by the entropy which, at least for the cases we have considered, seems to characterize...
the degree of equilibrium in an a priori highly non-equilibrium process such as an explosion. Now, more theoretical work needs to be done in order to understand why $\Sigma$ behaves in this seemingly interesting way.

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