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# Entropy puzzle in small exploding systems

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**Abstract**

We use a simple hard-core gas model to study the dynamics of small exploding systems. The system is initially prepared in a thermalized state in a spherical container and then allowed to expand freely into the vacuum. We follow the expansion dynamics by recording the coordinates and velocities of all particles until their last collision points (freeze-out). We have found that the entropy per particle calculated for the ensemble of freeze-out points is very close to the initial value. This is in apparent contradiction with the Joule experiment in which the entropy grows when the gas expands irreversibly into a larger volume.


Energetic nucleus–nucleus collisions open a unique possibility to study explosive dynamics of strongly interacting many-body systems in the laboratory. Highly excited matter produced in such collisions expands into vacuum until its constituents decouple (the freeze-out stage). There exist many models for describing this process which range from simple macroscopic to fully microscopic ones. Within thermal and fluid dynamical models it is usually assumed that the matter expansion is isentropic, i.e., proceeds at constant entropy. On the other hand, as well known from statistical physics [1], only slow reversible processes conserve entropy. It is known from the Joule experiment [2] that the entropy grows if the state of the system changes too fast. In this Letter we examine the entropy conservation hypothesis on the basis of a microscopic model.

For this study we employ a simple gas model where the constituent particles collide like billiard balls and follow the classical Newtonian dynamics. This model, first introduced for simulating heavy-ion collisions in Ref. [3], was recently applied [4] for investigating de-equilibration dynamics in expanding matter. We consider a gas of identical balls of radius $r_c$, which perform classical nonrelativistic elastic scatterings at impact parameters $b < 2r_c$ with conservation of energy and momentum. Rotational degrees of freedom of the balls are ignored. The initial system consists of $N$ such particles placed randomly within a sphere of radius $R$, rejecting configurations where particles overlap within the hard-core distance. The particle velocities are generated from a Gaussian distribution with variance $T/m$ where $T$ is interpreted as temperature. Then the particles are allowed to collide for a certain time ("cooking" stage) in order to fully equilibrate the system. For our simple interaction the total energy of

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the gas is obviously given by the ideal-gas relation $E = 3NT/2$ independent of gas density.

In our simulations we arbitrarily choose conventional nuclear scales: the mass of the constituent particle is $m = 940\ \mathrm{MeV}/c^2$, the hard core radius is $r_c = 0.5$ fm, and the initial radius of the gas sphere is $R = r_0 N^{1/3}$. Most simulations are performed with $r_0 = 1.2$ fm corresponding to the normal nuclear density $\rho_0 \approx 0.14\ \mathrm{fm}^{-3}$. To investigate the role played by the finite-size effects we have performed simulations for 4 systems, $N = 50$, 100, 200 and 400. This covers the range of baryon numbers actually achievable in heavy-ion collisions. The initial average energy $E_i \approx 118$ MeV per particle and the corresponding temperature $T_i \approx 78$ MeV were chosen to safely ignore quantum and relativistic effects. The characteristic sound velocity for an ideal gas at this temperature is $c_s \approx \sqrt{T/m} \approx 0,186c$.

When the gas is confined in a container the particles collide not only with each other but also with the container wall. When the container expands the gas particles loose energy and momentum while colliding with the moving walls. In the case of slow expansion these losses are rapidly redistributed over all particles and the gas remains in thermal equilibrium. This case corresponds to the reversible process when the temperature decreases with volume according to the adiabatic relation

$$TV^{\gamma-1} = \text{const}, \tag{1}$$

where $\gamma \approx 5/3$ is the adiabatic index. However, when the expansion is fast fewer particles reach the wall and the energy losses are smaller than needed for the adiabatic expansion. In the case of a very fast expansion of the container no particles can collide with the wall and therefore the energy of the gas remains constant. If the wall stops at a larger radius, the gas will eventually relax to a new equilibrium state in the larger volume. The relaxation time can be estimated as $\Delta R/c_s$. Since the total energy and accordingly the temperature is practically unchanged, the entropy of the equilibrated gas increases due to the larger volume, as expected for a fast irreversible process. This simple physics is behind the Joule experiment. Although the traditional Joule experiment was performed with nonspherical containers, the general principles are obviously valid for the spherical geometry considered in this Letter. Our simulations show that the transition from the slow to fast expansion is rather sharp and takes place at wall velocities of approximately $0.5\,c_s$.

More difficult problems arise when gas or fluid expand into the vacuum without any container. The question which we want to address is whether the expanding matter itself generates a sort of wall effect which may simulate an isentropic process. This question is closely related to the problem of freeze-out and collective flow in exploding systems. The simplest scenario which is often used in the literature is to say that the system expands isentropically until all interactions between the constituents cease. Then the change in the internal energy of the matter is transferred into a collective flow energy. But the problem is that the freely expanding system has no well-defined volume. In our previous study [4] we have defined the instantaneous volume by taking a high, 20th, moment of the particle spatial distribution. For each time step we have defined the entropy as $S = -\sum_k p_k \ln p_k$ where $p_k$ is the occupation probability of the phase space cell $k$ in the comoving grid. This entropy was compared with a reference entropy $S_{\mathrm{ref}}$ defined for the equilibrated system of the same volume. From simulations at different initial conditions for a system of 50 particles we have found that the equilibration measure $\Sigma = \exp(S - S_{\mathrm{ref}})$ at late times was not equal to 1 but rather close to 0.6.

Below we adopt a slightly different strategy using the microscopic information on the freeze-out field. The initial state is prepared in the same way as before but now after a "cooking" stage the container wall is completely removed and the gas is allowed to expand freely into the vacuum. It is important to stress that this free expansion starts from a state with well-defined temperature and density. All particles are followed until their last collision when their coordinates and momenta are recorded. For each system we generate many such events and define the freeze-out field as the set of all such coordinates and momenta. As demonstrated in Ref. [4], these fields are nonlocal in space and time, in contrast to a simplified Cooper–Frye picture [6] assuming a sharp freeze-out hypersurface. We point out also that the number of freeze-out points per event is generally less than the number of particles because some particles leave the system without any collision (see Table 1).

After obtaining the freeze-out field we calculate the average characteristics of the phase space occupation.

Table 1
In this table, $n_{\text{event}}$ is the number of events, $n_{\text{freeze}}$ is the number of freeze-out points, $F_{\text{freeze}}$ is the freeze-out fraction defined in the text, $s_{\text{inital}}$ and $s_{\text{final}}$ are the inital and final entropy per particle, respectively. Notice that the freeze-out fraction increases with system size, and that the final freeze-out entropy per particle approaches the inital value for larger systems

| $N$ | $n_{\text{event}}$ | $n_{\text{freeze}}$ | $F_{\text{freeze}}$ | $s_{\text{initial}}$ | $s_{\text{final}}$ |
|---|---|---|---|---|---|
| 50 | 128 | 3848 | 0.60 | 2.68 | 3.27 |
| 100 | 64 | 4388 | 0.69 | 2.69 | 3.07 |
| 200 | 32 | 4673 | 0.73 | 2.71 | 2.97 |
| 400 | 16 | 5048 | 0.79 | 2.70 | 2.75 |

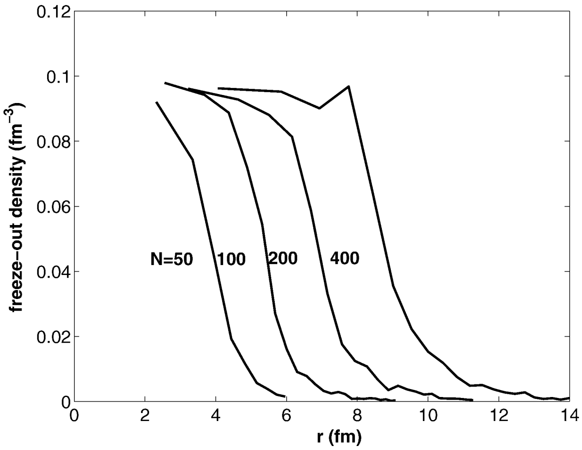


Fig. 1. Radial density of freeze-out points for free expansion of the gas spheres with $N = 50$, 100, 200 and 400. The initial temperature 78 MeV and density 0.14 fm$^{-3}$ of the gas are the same in all cases.

Utilizing spherical symmetry of the system we divide it into a number of spherical shells of radii $R_k$. For each shell we calculate the average density of freeze-out points $\rho(r)$, collective velocity $u(r)$ and temperature $T(r)$. The collective velocity is defined simply as the mean radial velocity of frozen-out particles in a given shell, i.e., between $R_k$ and $R_{k+1}$,

$$u(r) \equiv \bar{v}(r) = \frac{1}{N_k} \sum_{i=1}^{N_k} v_r(\mathbf{r}_i), \tag{2}$$

where $N_i$ is the number of freeze-out points in this shell, $\sum_k N_k = N$. The temperature is determined from the variance of velocities in the shell, assuming the ideal-gas relation,

$$T(r) = \frac{m}{3}\left(\overline{v^2}(r) - \bar{v}^2(r)\right), \tag{3}$$

and the mean-square velocity is defined in the standard way,

$$\overline{v^2}(r) = \frac{1}{N_k} \sum_{i=1}^{N_k} v^2(\mathbf{r}_i). \tag{4}$$

With this information in hand we can calculate the final entropy of the gas. Since at this late stage of expansion the gas is very dilute one can use the ideal-gas formulae. The freeze-out entropy in a given shell is defined as

$$S(r) = N_k \ln\left[\frac{V_k e^{5/2}}{N_k \lambda_T^3}\right], \quad \lambda_T = \left(\frac{2\pi\hbar^2}{mT(r)}\right)^{1/2}, \tag{5}$$

and the total entropy is obviously given by the sum over the shells. We believe that this definition of entropy is valid despite the fact that it is applied not to the real gas but to the ensemble of freeze-out points in the phase space. Here one can use an analogy with the microwave background radiation in the Universe which keeps its entropy constant despite the fact that the photons have decoupled from the matter at the recombination stage a long time ago.

To make statistical errors similar for different systems, the number of generated events is chosen to be inversely proportional to the system's particle number (see Table 1). This guarantees that the total number of freeze-out points is approximately the same for all considered systems. The dynamical simulations were performed with the time step of 0.5 fm$/c$ which was sufficient to resolve practically all collisions.

The results of the simulations are presented in Figs. 1–4 and Table 1. Because of the limited statistics the spatial distributions shown in the figures are sensitive to the binning of data. Most calculations were done by sampling freeze-out points in spherical shells of equal volume ($r^3$ binning). This guarantees uniform statistical errors for the bulk parts of distributions but leads to enhanced fluctuations on their tails. Moreover, for unambiguous separation of flow and thermal components the radial bin size should be sufficiently small.

It is necessary to emphasize that the spatial characteristics presented in Figs. 1–4 correspond to sampling of freeze-out points irrespective of the times when particles have actually decoupled from the system. They represent the whole freeze-out history and in this re-

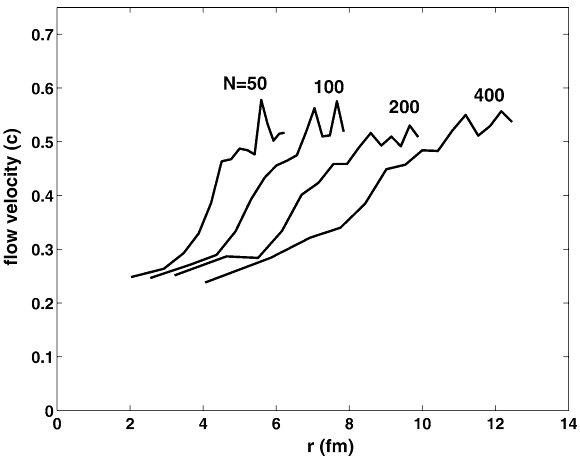


Fig. 2. Radial profiles of the collective velocity at freeze-out. Notations are the same as in Fig. 1.

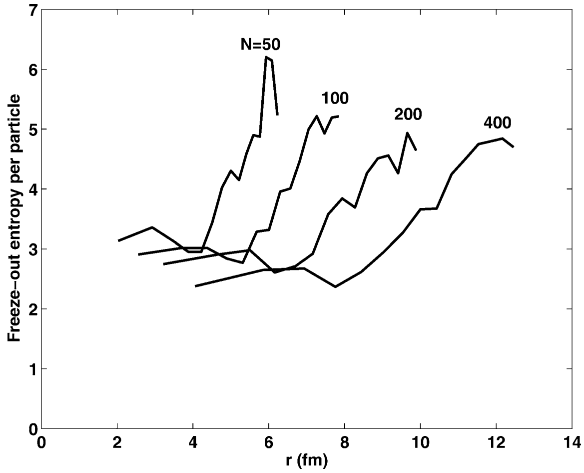


Fig. 4. Radial distribution of the entropy per particle at freeze-out. Notations are the same as in Fig. 1.

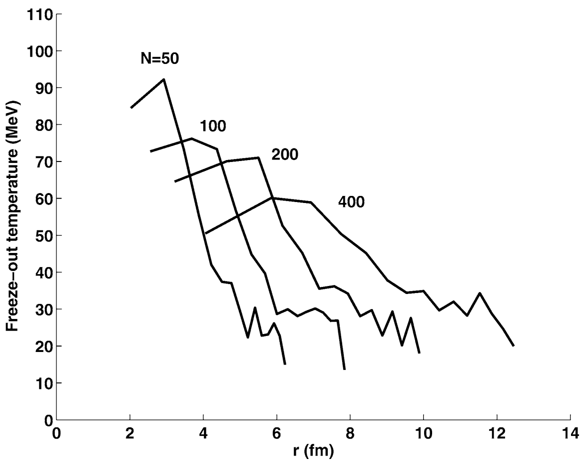


Fig. 3. Radial profiles of the temperature at freeze-out. Notations are the same as in Fig. 1.

spect differ from the time evolution of the gas characteristics usually presented in gasdynamical calculations. We believe that this representation is more adequate for calculating observable characteristics of small exploding systems. This is especially true for the interpretation of experimental data on energetic nucleus–nucleus collisions.

Fig. 1 shows the spatial density of freeze-out points averaged over all events. In all cases it has a bulk part and a tail. The bulk density is about 0.1 particles/fm$^3$ and almost independent of the system. This should be compared with an initial density of 0.14 particles/fm$^3$. In the tail region the density rapidly drops to zero over a radial distance of about 2–3 fm. Such behavior should be anticipated from the general consideration of the freeze-out process [6]. The tail is formed by particles emitted through the surface at early times and the inner part contains particles from the bulk freeze-out.

Fig. 2 presents the collective velocity profiles calculated on the freeze-out fields. With a certain degree of imagination one can recognize a Hubble-like behavior. As expected the collective velocity grows to the outer edge of the distribution. The peak value of about 0.5–0.6 is reached somewhere in the tail region. This value is in good agreement with gasdynamical calculations [5] predicting for leading particles a velocity of about $3c_s$.

The temperature profiles presented in Fig. 3 are in a certain sense complementary to the flow profiles. One can see that the temperature reaches maximum values at the edge of the bulk region and these values decrease progressively with the system's size. This can be explained by the fact that the freeze-out process in larger systems develops at later stages of expansion leading to lower freeze-out temperatures. As well known (see, e.g., Ref. [5]), in a macroscopic system the freeze-out temperature approaches zero and the whole thermal energy is finally transformed into collective flow. We clearly see the transition from "small" to "large" systems by analyzing the average number of collisions per particle. As we see from our simulations, this number scales roughly as $\sqrt{N}$. While it is only about 1 for $N = 50$ (small system), it is already 2–3 for $N = 400$ (mesoscopic system), and will be about 10 for $N = 5000$ (large system).

Finally we come to the most interesting quantity, i.e., the entropy per particle as defined by Eq. (5). Fig. 4 shows the corresponding profiles. One can see two clear features. First, the entropy per particle is rather constant over the bulk region and its value varies very little with the system size. Second, there is a significant rise in the entropy per particle in the tail region well above the bulk value 2–3. Moreover, the smaller the system the stronger the rise. This latter trend can be explained by the bigger volume per particle in the outer tail region.

Now we can go back to our discussion of entropy conservation. For this analysis we use the total entropy per particle calculated at freeze-out and compare it with the initial entropy. The latter is calculated by applying the same Eq. (5) for the whole gas in the initial volume. The results are presented in Table 1 together with the number of particles, the number of events, the total number of freeze-out points for each size ($N$) and the freeze-out fraction $F_{\text{freeze}} = n_{\text{freeze}}/(Nn_{\text{event}})$.

From Table 1 one can see that surprisingly enough the initial and final entropies per particle are rather close to each other in all cases. The increase of about 0.5 units is largest for the smallest system considered ($N = 50$). Formally this is a 20% effect which is quite significant. However, one should bear in mind that in classical statistics the absolute value of entropy is defined up to a constant. This increase in entropy for small systems is an effect of the surface of the system: as seen from Fig. 4, the entropy per particle increases significantly with radius, and since there is relatively more surface in a small system also the total entropy per particle is bigger.

One may wonder, if entropy per particle is conserved, what happens to the total entropy of the system? Indeed, a significant fraction of particles ($1 - F_{\text{freeze}}$) leaves the system without scatterings. The simulations show that these "missing" particles are emitted early in the expansion and come predominantly from the surface region. We have not analyzed their characteristics in detail but we know that these particles were initially in thermal equilibrium with the rest of the system. Thus they should carry away approximately the same amount entropy per particle as in the initial state. Therefore, we expect that the total entropy of the system is also approximately conserved.

In conclusion, we have used a simple model for a repulsive gas to study the explosive dynamics of small systems. We have demonstrated that in the course of free expansion the temperature drops and collective flow develops in the gas. In contrast to our expectations we have found that the entropy per particle defined on the freeze-out field is almost conserved even in systems with a few hundred particles. This justifies the application of thermal and hydrodynamic models for describing matter evolution in energetic collisions of medium and heavy nuclei. Based on these results we put forward a new interpretation of the old Joule experiment. The gas expansion in this case is approximately isentropic at freeze-out before the particles hit the wall. Then the entropy is produced while the system equilibrates in the larger volume.

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