THERMODYNAMICS - A VALUABLE APPROACH TO MULTIFRAGMENTATION ?

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Thermodynamics - a valuable approach to multifragmentation?

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Abstract

Since years it has been vividly debated whether multifragmentation is a thermal or a dynamical process. Recently it has been claimed [1, 2] that new data allow to decide this question. The conclusion, drawn in these papers, are, however, opposite. Whereas [1] states that the behavior of different observables as a function of the fragment multiplicity excludes a thermal origin of the fragments in [2] it has been argued that data show a first order phase transition between a liquid and a gaseous phase. It is the aim of this paper to show that both conclusions are premature. They are based on the salient assumption, that the system is sufficiently large to be susceptible to a canonical description. We will show that this is not the case. A micro canonical approach describes the data as good as dynamical calculations. Hence the quest for the physical origin of multifragmentation continues.

1 Introduction

Since almost a decade the study of multifragmentation characterized by the multiple production of intermediate mass fragments ($3 \leq Z \leq 20$) is one

of the central issues in intermediate energy heavy ion collision studies. For beam energies in between 50A MeV and 400A MeV multifragmentation has been identified as the dominant reaction channel and up to 15 intermediate mass fragments (IMF's, $Z \geq 3$) have been observed in a single event.

The mechanism of multifragmentation, however, remained rather debated because the different mechanisms proposed predict the same functional dependence for several key observables. If the disintegration of the nucleus is instantaneous each nucleon keeps its momentum and one expects an average fragment kinetic energy of $3/5E_F$ [3] independent of the fragment size , where E_F is the Fermi energy. The same independence one expects if the fragments are formed very late, after the system has been expanded while maintaining thermal equilibrium. This requires that the disintegration is very slow. Here the average kinetic energy is 3/2 T, where T is the temperature at freeze out. The same ambiguity one finds for the mass yield where thermal[6] and non thermal systems [4, 5] show the same form. Hence more complicated observables have to be employed to distinguish between the different possible reaction mechanisms.

Recently it has been conjectured by Tõke et al. [1] that one can distinguish between a statistical process and a dynamical process by investigating several observables as a function of the fragment multiplicity. In analyzing their data, obtained in their limited acceptance region, they made the following observations:

1. The average transverse kinetic energy of the intermediate mass fragments (IMF's) is independent of the number of observed fragments.

2. The average light charged particle (LCP) multiplicity as well as the total kinetic energy of the LCP's is also independent of the number of observed fragments.

They considered this observation as contradictory to the assumption that the system is in equilibrium and argue as follows: Independent of the unknown impact parameter b the energy per nucleon and hence the temperature in the center of mass is almost identical. By varying b one changes the size of the source but not its temperature. Indeed, the observed average kinetic energy of the LCP's is independent of the number of IMF's. If the temperature of the system is constant in thermal equilibrium the ratio between LCP's and IMF's is determined by the chemical potential and hence fixed. Thus the increase of the particle number (sum of free nucleons and those entrained in

fragments) in the observed phase space interval has to be shared between the fragments and the free nucleons. Due to 2.) this is obviously not the case.

The opposite conclusion has been drawn from the analysis of experimental data by [2]. In this paper it is the isotopic yield ratio of fragments which is used to determine the temperature of the systems. Plotted as a function of the excitation energy of the system the temperature shows a plateau. The claim that the system is in thermal equilibrium is based on the similarity of this observation with the latent heat observed in a first order phase transition in infinite systems.

Both interpretations of the experimental data rely on the assumption that the equilibrated source is sufficiently large to be treated as a canonical system. It is the first purpose of this article to show that this salient assumption is not justified. Using a microcanonical statistical model [7] we reproduce the results of ref. [1]. This renders their conclusions premature. Taking the temperature fluctuations in finite size systems seriously we will show that the variance of the temperature distribution is not negligible and hence one cannot distinguish between a constant and an increasing temperature as a function of the excitation energy of the system. Furthermore the temperature fluctuations give rise to a nontrivial relation between the apparent temperature measured by the fragment yields and the temperature of the emitting source. Thus the conclusions of ref.[2] that data show an allusion of a first order phase transition are premature as well. The experimental determination of the mechanism which causes multifragmentation remains to be a challenge.

The second purpose of this article is to show that microcanonical statistical models predict strong correlations for systems as small as those observed in heavy ion reactions.

The third purpose is to show that - even worse - the observables discussed in ref. [1] do not allow to distinguish between a dynamical and a statistical reaction scenario. For that purpose we compare the results of the microcanonical statistical model [7] with those obtained by Quantum Molecular Dynamics simulations [8]. The analysis of the latter shows a nonstatistical origin of the fragments[9, 11, 10] (although the model itself is able to follow the evolution of a system towards equilibration if there were any).

2 Microcanonical and Canonical Systems

Before we start out with the detailed calculation a reminder on the differences between the microcanonical and the canonical approach to study systems in equilibrium is appropriate. For this discussion we will be guided by the question at hand: what can we learn about the system by analyzing observables measured in a subsystem. This subsystem may be the limited part of the phase space which is free from a contamination by preequilibrium emission or may be the ensemble of fragments in experiments where nucleons cannot be measured. This question can be discussed best if we divide the system, which is characterized by its macroscopic parameters, the energy E, the particle number N and the volume V, into two parts, the observable and the unobservable part of phase space.

A microcanonical description of an equilibrated system is based on the assumption that in statistical equilibrium each microstate which is compatible with (E,V,N) is occupied with the same probability. $g_{obs}(E_{obs}, V_{obs}, N_{obs})$ is the number of microstates available in the observable sector which is characterized by $(E_{obs}, V_{obs}, N_{obs})$. The number of microstates of the whole system is consequently

$$G(E,V,N) = \sum_{N_{obs}} \sum_{E_{obs}} g_{obs}(E_{obs}, V_{obs}, N_{obs}) \cdot g_{unobs}(E - E_{obs}, V - V_{obs}, N - N_{obs}). \tag{1}$$

V_{obs} is considered as constant here. The entropy of the system is given by $S^{mc} = k\ log\ G(E,V,N)$ (k being the Boltzmann constant) whereas the entropy of the observable subsystem is $S^{mc}_{obs} = k\ log\ g_{obs}(E_{obs}, V_{obs}, N_{obs})$. Knowing the functional dependence of S on E and N we can easily calculate the temperature $1/T = \frac{\partial S}{\partial E}$ and the chemical potential $\frac{\mu}{T} = \frac{\partial S}{\partial N}$. For the combined system with

$$G(N, E, E_{obs}) = \sum_{N_{obs}} g_{obs}(N_{obs}, E_{obs}) g_{unobs}(N - N_{obs}, E - E_{obs}) \tag{2}$$

one finds

$$\frac{k\partial\ lnG}{\partial E_{obs}} = \sum_{N_{obs}} \frac{k\partial\ lng_{obs}(N_{obs}, E_{obs})}{\partial E_{obs}} + \frac{k\partial\ lng_{unobs}(N - N_{obs}, E - E_{obs})}{\partial E_{obs}} \tag{3}$$

$$= \sum_{N_{obs}} \frac{k\ \partial\ lng_{obs}(N_{obs}, E_{obs})}{\partial E_{obs}} - \frac{k\ \partial\ lng_{unobs}(N - N_{obs}, E_{unobs})}{\partial E_{unobs}} \tag{4}$$

$$= \sum_{N_{obs}} \frac{1}{T_{obs}} - \frac{1}{T_{unobs}} \tag{5}$$

For fixed values of E,N we may find in the both subsystems different values E_{obs}'s and N_{obs}'s and consequently a distribution of T_{obs}'s and μ_{obs}'s. Only at the maximum $\frac{k\partial lnG(N,E,Eobs)}{\partial E_{obs}} = 0$ the temperatures in both subsystems agree. Therefore generally it is not possible to infer from the temperature, chemical potential, particle number or energy of the observable subsystem the corresponding values of the whole system or the other subsystem and vice versa.

This is of course completely counterintuitive because from daily life we are used to large systems. Because for a given energy of the total system the fluctuations of the temperature in a subsystem are $\propto \frac{1}{\sqrt{N}}$, where N is the number of particles in this subsystem, in macroscopic systems the fluctuations of the temperature can be neglected. In other words, if the system is sufficiently large $(E \to \infty, N \to \infty)$ $g_{obs} \cdot g_{unobs}$ is very sharply peaked and the sums in eq. 1 can be replaced for all practical purposes by the largest term. Then the entropy becomes additive and the temperatures and chemical potentials in the subsystems are identical. Under this condition the microcanonical and the canonical calculations coincide. If this is not the case the (isolated) system is not susceptible to a canonical but only to a microcanonical treatment.

For the interpretation presented in [1, 2] it is crucial that the system is large and energetic enough to justify a canonical treatment. In ref. [1] the observed subsystem can be identified with the limited acceptance region of the experiment, in ref.[2] with the subsystem of fragments which is used to determine the apparent temperature. It is this apparent temperature which has a plateau as a function of the excitation energy of the equilibrated source.

To verify if the nuclear system is sufficiently large to justify a canonical description we employ one of the state of the art statistical models, the Statistical Multifragmentation Model (SMM), which has been developed by the Copenhagen group and has later been improved by Botvina [7]. There all possible microstates of the nuclear system are carefully elaborated. This model has been employed frequently to interpret heavy ion reaction data. It suffers, however, as every model of this kind, from 3 unsolved problems: a) from the problem how to treat particle unstable nuclear levels, b) from the not well known level density at large excitation energies and c) from the fact that there is no experimental information on the freeze out volume. The

results of statistical model calculations depend on the proposed solution of these problems [13]. Therefore, to study the conjecture of [2], where this problem becomes crucial, we employ in addition a simpler microcanonical model which allows for an analytical solution. It serves as well the purpose to understand qualitatively the fluctuations observed in the SMM calculations. For a general introduction to the statistical physics of multifragmentation we refer to ref.[12].

3 Comparison with data

For our studies we use data and simulations for central collisions of the reaction 50A MeV Xe + Sn where precise data are available, taken by the INDRA collaboration[14, 15]. Both models, SMM and QMD, have been extensively used to interpret this reaction [11, 14]. As said the analysis of the QMD calculations shows that in this approach the system never passes through a state of thermal equilibrium [9, 10] whereas the application of SMM is only justified if such a state is formed. Thus the reaction scenarios in these models are orthogonal. For the comparison with the data both calculations have been filtered with the experimental acceptance. To model the centrality it turns out [11] that one has to require for the (filtered) QMD simulations that the total transverse energy of LCP's is larger than 450 MeV. For the statistical model calculations we use a slightly different centrality cut. For a comparison of both cuts, whose difference is of no importance here, we refer to ref. [11]. The increase of the average transverse energy of the fragments as a function of their mass, observed in the experiment, is larger than predicted in SMM [14] calculations. Therefore one has to modify the statistical model calculations by adding a fourth system parameter, a collective energy, which is parameterized as $E_{coll} = c * A$, where c is a parameter which remains to be determined and A is the fragment mass. The best agreement between experiment and SMM calculation is obtained with the following set of input parameter:

freeze out density:	$1/3\rho_0$
source size:	Z_S=78 A_S = 186
excitation energy:	$E_{thermal}$=7A MeV E_{coll}=2.2A MeV

Even central collisions at intermediate energy have a binary character [11] and consequently emission of particles from residues close to beam or target velocity spoils the spectra of particle emission from a possible thermal source at rest in the center of mass. Therefore a meaningful comparison between statistical model calculations and experimental data is only possible around $\theta_{CM} = 90^o$. We subdivide the experimental data and the QMD simulations into two equal size 2π intervals:

$$B_{obs}: \quad 60^o \leq \theta_{CM} \leq 120^o$$
$$B_{unobs}: \quad \theta_{CM} < 60^o, \theta_{CM} > 120^o.$$

In B_{obs} we observe a flat angular distribution and a constant average energy of IMF's and LCP's [15] as a function of the emission angle, both being prerequisites for a statistical equilibrium. In B_{unobs}, on the contrary,in the thermals language a preequilibrium component is superimposed to the thermal component. QMD which does not separate the phase space into two contributions but gives an continuous distribution for all observation angles describes this region well [11].

The theoretical as well as the experimental fragment energy distributions show an exponential shape. In fig. 1 we display on top the slope of the kinetic energy spectra of the fragments. The inverse slopes T are converted into an energy. On the bottom we show the charge yield distribution. We display the results for QMD and SMM calculations in comparison with the INDRA data. As one can see, these are well reproduced in both theories, underlining the above mentioned observation that these observables are not sensitive to the reaction mechanism.

In figure 2 we plot for B_{obs} different observables as a function of the IMF multiplicity. The left column displays the experimental results for the central reaction 50 AMeV Xe + Sn as measured by the INDRA collaboration.

In the first row we display the LCP multiplicity as a function of the number of observed IMF's. At higher energies, where the number of LCP's is much larger, the LCP multiplicity is frequently considered as a measure for the centrality of the reaction (what is confirmed by the QMD calculations). As can be seen from the panel, in our case the multiplicity of LCP's is independent of the IMF multiplicity. Thus one may conjecture that the (central, $E_{trans} \geq 450\ MeV$) events with different IMF multiplicities in B_{obs} have the same average impact parameter. Also the average kinetic energy of LCP's and IMF's, displayed in the second row, is independent of the number of IMF's. The third row displays the sum of the kinetic energies of the IMF's and LCP's, respectively. We observe, as expected from row 1 and

2, a constant value for the LCP's and a linear increase for the IMF's. The fourth row displays the total kinetic energy in B_{obs} divided by the sum of the number of LCP's and IMF's. In a canonical system of noninteracting particles this quantity is related to the temperature by $T = \frac{2}{3}\frac{E}{N}$. We see that the average value decreases with decreasing fragment number and the fluctuation are considerable ($< \Delta E/\overline{E} >= \sqrt{\overline{E^2} - \overline{E}^2}/\overline{E} = 0.2$). The fourth row shows as well the total number of nucleons (free or as part of the fragments) in B_{obs}. It varies by almost a factor of 3 although the number of LCP's stays constant.

These observations, although presented here for another reaction, agree well with the findings of ref. [1]. Thus, if their arguments were valid, we would arrive at the same conclusion.

However, we are dealing with a rather small system. Fluctuations between B_{obs} and B_{unobs} may be important and hence the system may be too small for a canonical description. To see whether this is true we performed the same analysis using the microcanonical statistical model. The results are presented in the second column of fig. 2. We see that the statistical model results agree well with experiment. The results are, however, quite different from those of a canonical description of the data. There μ and T are identical in both subsystems once E,N,V are given and so is the ratio between IMF's and LCP's which is fixed by the chemical potential. Thus fluctuations (between the two small subsystems B_{obs} and B_{unobs}) and correlations (due to the conservation of N and E) are not only important but essential for the results.

Does this result mean that data prove that multifragmentation is a statistical process? To answer this question we performed calculation with QMD [8] The results are presented in the third column. Besides of the too small average fragment energy (which is a consequence of a shortcoming of QMD, the artificial long range of the attractive nuclear potential which suppresses the Coulomb repulsion [8] and therefore decreases the average fragment energy) also the results of QMD agree in the error bars with those of experiment.

Thus we arrive at the conclusion that even this quite involved analysis of the fragment production does not allow to distinguish between a statistical and a dynamical origin. One should keep in mind, however, that QMD is able to describe both, B_{obs} and B_{unobs}, whereas a comparison with SMM is limited to B_{obs} because in B_{unobs} nonstatistical processes dominate the fragment production.

How the correlations in the statistical model calculation show up in detail is shown in fig. 3 where we display the SMM results before filtering. The upper panel shows the fragment multiplicity in 4π and in B_{unobs} as a function of the fragment multiplicity observed in B_{obs}. Of course, without filtering B_{obs} and B_{unobs} are two arbitrary 2π bins which should not differ. However, we observe strong correlations between the fragment multiplicities in the two 2π intervals. In the lower panel we compare the true fragment multiplicity distribution in 4π with that obtained by a convolution of the multiplicity distribution observed in one 2π subsystem. If no correlations were present we would expect for 4π a convolution of the distribution observed in 2π. This is obviously not the case and consequently it is impossible to infer in systems as small as this the multiplicity distribution in 4π from a 2π subsystem.

4 Temperature fluctuations in a small system

To address the conjecture of the second paper [2] it is important to now the temperature fluctuations in the relevant subsystem under the condition that the total energy of the system is constant. This question is not easy to address because the relevant subsystem is the environment of those fragments which are used to determine the temperature by calculating isotope ratios. This information is not available in SMM. Therefore we assume that the temperature fluctuations of the subsystem consisting of the intermediate mass fragments $Z \geq 3$ is a good measure for those of the above mentioned observable. We use the above mentioned microcanonical SMM calculations and identify the two subsystems with the fragments with $Z \geq 3$ and the LPC's, respectively. To calculate the temperature fluctuation we employ eq.3.

In fig. 4, top, we display the number of events (left) and the average number of IMF's (right) as a function of the total number of nucleons entrained in the fragments and the total fragment energy. We see a rather broad distribution. In the middle we present the difference of the temperatures and of the chemical potential in the two subsystems (LPC's and IMF's) as a function of the total mass and the total energy of all IMF's. For calculating the temperature difference we have assumed that $\frac{1}{T_1} - \frac{1}{T_2} \approx \frac{\Delta T}{T^2 + \Delta T^2/4}$ where T is assumed to be 7 MeV. We see a rather broad distribution of the chemical potentials and of the temperatures. The probability distribution of fragments to be emitted in a microstate which shows a $\mid \Delta T \mid$ and a chemical potential difference of $\mid \Delta\mu \mid$, respectively, between the two subsystems is plotted in the

bottom row. The chemical potential $\mid \Delta\mu \mid$ in units of the temperature fluctuates by about to 40% around the mean value 0 whereas the variation of the distribution of the temperature difference between the subsystems is about 1.7 MeV. More precisely the temperature in the subsystem of the fragments cannot be determined.

To show that these results are generic and do not depend decisively on the mentioned problems of these microcanonical statistical model approaches we employ a much simpler model to confirm the order of magnitude of the above result. It has the advantage that is allows for analytical results. Although this model neglects the long range Coulomb force which make thermodynamics much more complicated it is sufficiently realistic to understand the physical origin of the fluctuations.

We consider a noninteracting system consisting of N_F fragments and N_N free nucleons. The energy $E = E_F + E_N$ of the system is constant. We calculate the fluctuation of the total fragment energy and hence the fluctuation of the temperature if only fragments are measured. The temperature of the whole system is fixed once density , particle number and total energy are given.

The probability to have a total fragment energy E_F is proportional to the available number of microstates for this division of the energy:

$$P(E_F, \rho, N_F) = \frac{e^{S(E_F,\rho,N_F)/k + S(E-E_F,\rho,N_N)/k}}{e^{S(E,\rho,N_F+N_N)/k}}. \tag{6}$$

Assuming that we can use the ideal gas entropy

$$S(E, \rho, N) = Nk(\frac{5}{2} + ln(\frac{\rho}{h^3}(\frac{4\pi mE}{3N})^{\frac{3}{2}})) \tag{7}$$

the probability to find an energy fraction of E_F/E for the total energy of the fragments is given by

$$P(x = E_F/E, N_F, N_N) = \frac{\Gamma(2 + \frac{3N}{2})}{\Gamma(1 + \frac{3N_F}{2})\Gamma(1 + \frac{3N_N}{2})}(1-x)^{3N_N/2} x^{3N_F/2} \tag{8}$$

where N $= N_F + N_N$. For the standard deviation of the energy $\Delta E_F = \sqrt{\overline{E_F^2} - \bar{E_F}^2}$ we find

$$\frac{\Delta E_F}{E} = \sqrt{\frac{3N_F+2}{3N+4}\frac{6(N-N_F)+4}{(3N+6)(3N+4)}} \quad ; \quad \frac{\Delta E_F}{\overline{E}_F} = \frac{\Delta T_F}{T_F} = \sqrt{\frac{6(N-N_F)+4}{(3N_F+2)(3N+6)}}. \tag{9}$$

For central reactions 50A MeV Xe+Sn we have typically $N_N = 50$ and $N_F = 8$. Thus we find $\frac{\Delta T_F}{T_F} = 0.24$ and hence about the same value as in the SMM approach. Thus the order of magnitude of the fluctuation is given by the size of the system only and does not depend on the details of the Hamiltonian or the freeze out volume.

This has consequences for the value of the apparent temperature measured by an isotope ratio. Because the isotopic yield ratio depends exponentially on the temperature ($\frac{P_1}{P_2} \propto exp - (E_1 - E_2)/T$) the mean value of the apparent temperature $T_{app} = (E_2 - E_1)/\ln < \frac{P_1}{P_2} >$, where $< \frac{P_1}{P_2} >= \int dT f(T) \frac{P_1}{P_2} / \int dT f(T)$, differs from the mean value $< T >$ of the temperature distribution f(T) in the subsystem of the fragments. On the other hand the apparent temperature is bounded from above because above a critical temperature between 6 and 8 MeV, depending on the microcanonical program, fragments are not stable anymore [17]. Therefore the increase of the apparent fragment temperature is smaller than that of $< T >$. That may be the origin of the observation that the mean value of the apparent temperatures increases slowly with increasing excitation energy.

Consequently, the argument, that the experimental data present evidence that in nuclear reactions a liquid gas phase transition can be observed, which was advanced in ref. [2], has two shortcomings. First, the temperature of the system extracted from the isotope ratios has large error bars, and hence it is not possible to distinguish between an (expected) increase of the temperature with beam energy and a constant value (which has been interpreted as sign of a latent heat). Second, the nonlinearity of the isotope ratio with temperature in connection with upper limit due to the instability of the fragments limits the apparent temperature to a small interval. Its dependence on the excitation energy of the system is small as compared to that of the mean value of the temperature distribution of the subsystem.

5 conclusions

First of all we have found that the nuclear systems of the size as expected to be formed in heavy ion reactions are too small to be susceptible to a canonical description but have to be analyzed in microcanonical approaches because the results of both approaches differ substantially.

Therefore, the conjecture of Toeke et al. that the functional dependence of the kinetic energies of fragments and light charged particles on the ob-

served number of IMF's may be used to distinguish between a statistical and a dynamical reaction mechanism, which was based on a canonical description, cannot be substantiated by detailed calculations. On the contrary, dynamical and microcanonical calculations give almost identical results. QMD calculations predict that the reaction never comes to a statistical equilibrium and is completely determined by the dynamics [9, 11]. Hence for a decision upon the reaction mechanism one has to study other observables.

Another result of the microcanonical analysis is the observation of large fluctuations of the temperature if it is determined from fragments only. Consequently, due to the nonlinearity of the isotopic yield ratio as a function of the temperature and due to the fact that at high temperature, fragments do not survive, the apparent temperature measured from the isotopic yield increases slower as compared to the mean value of the temperature distribution of the fragments. In any case the relation between the apparent temperature and the true temperature $1/T = \frac{\partial S}{\partial E}$ is not trivial. Hence the apparent temperature can not serve as a measure for the system temperature. If the fluctuation of the temperature distribution are properly taken into account, it is impossible to distinguish between a first order phase transition (assuming it manifests itself in finite systems as a latent heat) and an increase of the apparent temperature with increasing beam or excitation energy. Thus also the claim that data present evidence for a first order phase transition is premature. These observations of our simple model remains valid also in the framework of microcanonical models as can inferred from a comparison of [17] and [18].

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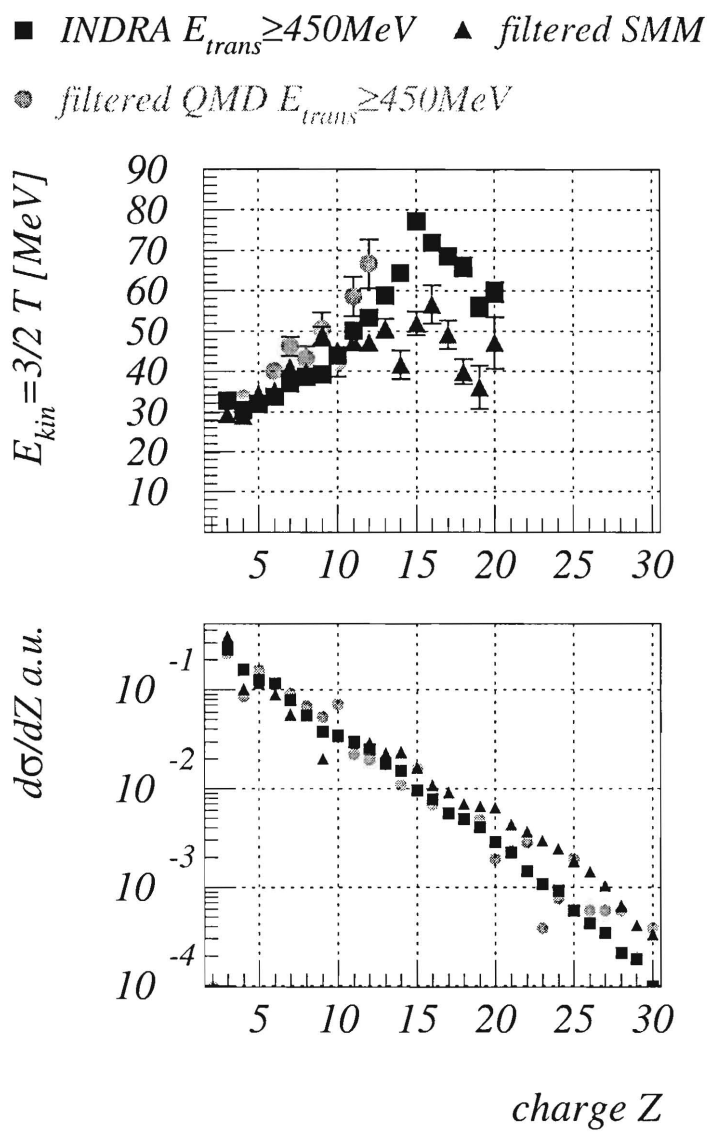

Figure 1: *Fitted slopes and the charge distribution for QMD, INDRA and SMM data in* $60^o \leq \theta_{CM} \leq 120^o$ *for 50A MeV Xe + Sn, central collisions.*

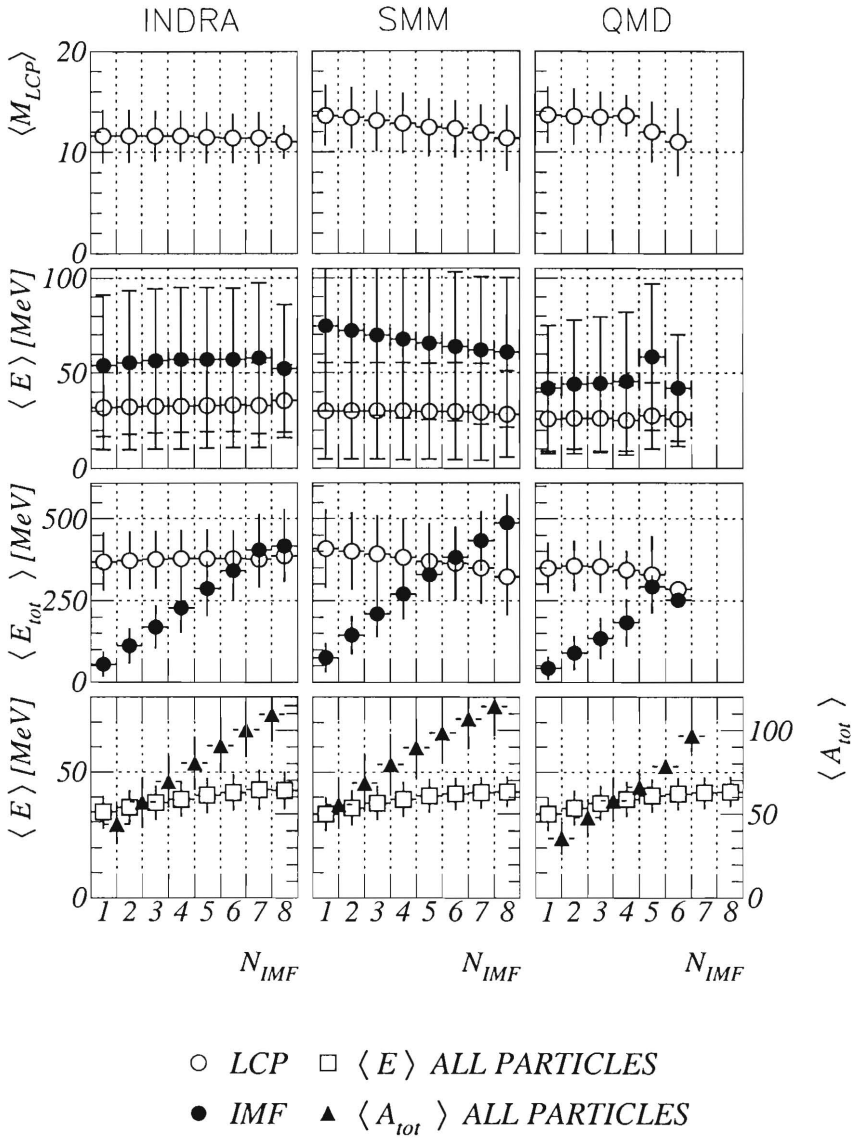

Figure 2: *As a function of the IMF multiplicity observed in* $60^o \leq \theta_{CM} \leq 120^o$ *we display for central events 50A MeV Xe + Sn several observables in* $60^o \leq \theta_{CM} \leq 120^o$*: The LCP multiplicity (top row), the average kinetic energy of IMF's and LCP's (second row), the total energy of IMF's and LCP's (third row), the average kinetic energy of all particles and the number of nucleons(forth row).*

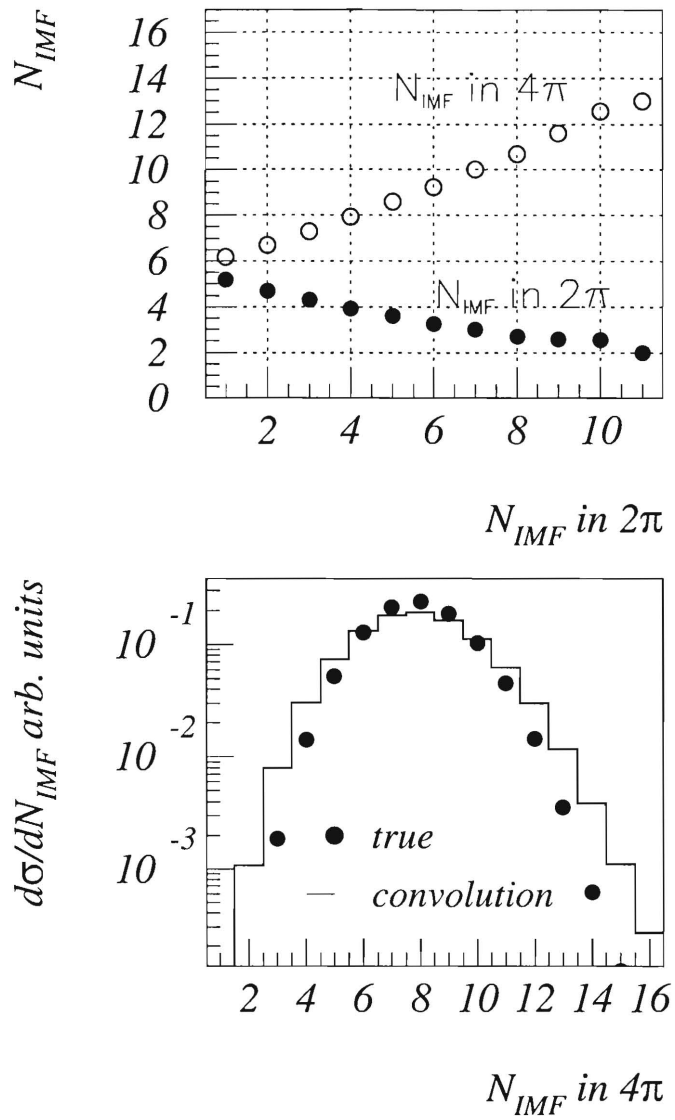

Figure 3: *Correlations as predicted by SMM calculation. We display the mean value of IMF's in the B_{unobs} and in 4π as a function of the fragment multiplicity in B_{obs} (top). Top right we display the actual IMF multiplicity distribution as compared to a convolution of the distributions observed in B_{obs} and B_{unobs}. The statistical model calculations are done for central reactions 50A MeV Xe + Sn*

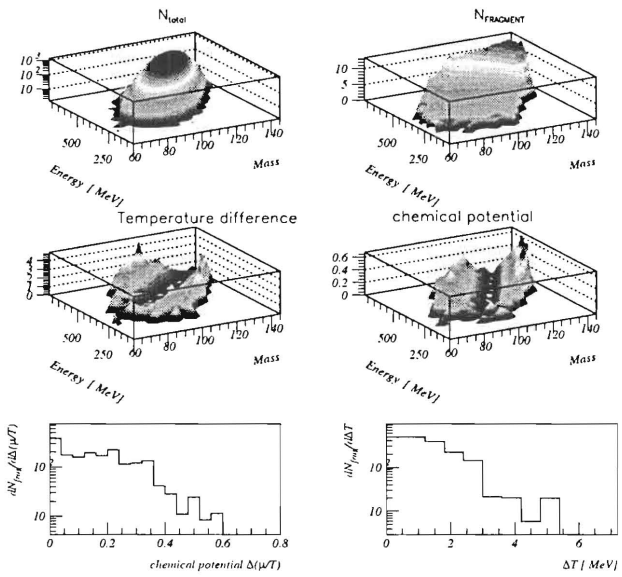

Figure 4: *Top: Number of events and number of fragments as a function of the total mass of all fragments and of their total energy. Middle: Distribution of the temperature difference and the difference of the chemical potential. Bottom: Distribution of the absolute value of the temperature difference distribution and that of the distribution of the difference of the chemical potentials between the subsystems formed by fragments and LPC's, respectively, for a SMM calculation adjusted to describe the INDRA results*