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Thermodynamics of Chaos

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(July 8, 1996)

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Abstract

We calculate the maximal Lyapunov exponents (LE) starting from concepts of hydrodynamics. Analytical expressions for the LE can be found in ergodic limit by using results of the classical thermodynamics for a Boltzmann gas and for systems undergoing a second order phase transition. We give a recipe to measure LE in systems which might have a critical behavior, such as a Bose-Einstein condensation or a transition to a quark-gluon plasma.

PACS numbers: 5.45+b, 5.70Fh, 47.52+j

In recent years, the ideas of a new branch of science commonly known as 'chaos', are raising more and more interest among scientist working in very different fields such as biology, physics, economics and others. Indeed, the idea that different complex systems might have something in common and are describable in terms of a simple 'map' is quite appealing [1]. An important quantity is the Lyapunov exponent (LE) which tells how much the nearby trajectories are separated after a time t. In particular, for positive LE two trajectories will separate exponentially and mixing of many such trajectories gives chaos, i.e. the impossibility of making predictions even if we know the initial conditions within a small uncertainty d_0.

These concepts have been widely applied to systems out of equilibrium, where a formal analogy between chaos and concepts of statistical mechanics has been worked out [2]. For equilibrated systems it is usually stated that the ergodic limit applies, i.e. time averages and ensemble averages are equivalent and one could calculate the LE from the statistical ensemble instead of the time averages [2]. However, for all ergodic systems which are well described by the classical thermodynamics, an explicit calculation of the LE, for instance from the equilibrium distribution, is still lacking. Here we will demonstrate that the maximal LE is proportional to the variance in momentum space of the final ($t \to \infty$) distribution. We will work out examples for a classical ideal gas and for a system undergoing a liquid gas phase transition. Our findings might have important consequences, in fact it could be possible to directly measure LE in experiments which provide final momenta distributions only.

To be more specific, let us define the relative distance between the two trajectories [2,3]:

$$d(t) = d_0 \, e^{\hat{\lambda} t} \quad , \tag{1}$$

as a function of time. The $d(t)$ can be expressed in terms of the phase-space variables:

$$d(t) = \left(\sum_{i=1}^{N} [a(\mathbf{r}_1(t) - \mathbf{r}_2(t))^2 + b(\mathbf{p}_1(t)) - \mathbf{p}_2(t))^2]_i \right)^{1/2} \quad , \tag{2}$$

where $\mathbf{r}, \mathbf{p}$ refer to the positions and momenta of N particles at time t. Indices '1' and '2' refer to the two trajectories differing by d_0 at $t = 0$. a, b are two arbitrary parameters which express the fact that the LE are independent of the particular metrics in the phase space [3]. The so called maximal LE is defined as :

$$\hat{\lambda} = \lim_{d_0 \to 0} \lim_{t \to \infty} \frac{1}{t} \frac{d(t)}{d_0} \quad . \tag{3}$$

Positive $\hat{\lambda}$ imply diverging trajectories while negative $\hat{\lambda}$ correspond to stable trajectories. To estimate LE, let us use the Navier-Stokes equation for the fluid velocitiy $u(x, y, z, t)$ [4] . For simplicity, let us consider an incompressible flow. The Navier-Stokes equation in this case reads:

$$\frac{\partial u}{\partial t} + u\nabla u = -\nabla p + \nu\nabla^2 u \quad , \tag{4}$$

where ν is the viscosity and p is the pressure divided by the density. Let u_0 and p_0 be some particular solution of the Navier-Stokes equation. Let us perturb this solution by a small amount :

$$u = u_0 + u_1$$

$$p = p_0 + p_1 \tag{5}$$

Clearly, u_1 is the distance in the velocity space between the new trajectory and the original trajectory. Inserting (5) in (4) gives :

$$\frac{\partial u_1}{\partial t} + u_0\nabla u_1 + u_1\nabla u_0 + u_1\nabla u_1 = -\nabla p_1 + \nu\nabla^2 u_1. \quad . \tag{6}$$

The solution of this equation has a time dependence as $e^{i\omega t}$. The frequencies ω are determined by solving eq. (6) with appropriate boundary conditions. These frequencies are in general complex. Positive values of the imaginary part reveal a steady damped oscillatory motion whereas negative values of the imaginary part of the frequencies reveal instabilities. Since we are interested in the case of fully developped chaos we will neglect purely oscillatory term in the solution and keep only exponentially increasing term. Thus, the perturbation to the steady velocity can be written as:

$$u_1 = d(t) f(x, y, z) \quad , \tag{7}$$

where $f(x,y,z)$ is some complex function of the coordinates and we have used the symbol $d(t)$ because it is proportional to the distance between two trajectories in the velocity space. Substituting (7) in (6) and grouping terms together gives:

$$\frac{\partial d}{\partial t}(t) = \gamma d(t) - \alpha d^2(t) \quad , \tag{8}$$

where α depends on the nonlinear term in u_1 and γ depends on the pressure, the velocity field as well as on the viscosity. Eq. (8) can be solved easily :

$$d(t) = \frac{d_\infty d_0}{d_0 + d_\infty e^{-\gamma t}} \tag{9}$$

$$\gamma = \alpha d_\infty \quad , \tag{10}$$

where $d_0 = d(t=0)$ and $d_\infty = d(t=\infty)$. In some cases (e.g. the ergodic limit), d_∞ equals the variance in the velocity space.

Eq. (9) has the interesting property of saturation for large times. For finite times, eq.(9) gives :

$$d(t) \approx d_0 e^{\gamma t} \quad . \tag{11}$$

Comparing eq. (11) with eqs. (1) and (10) gives :

$$\hat{\lambda} = \gamma = \alpha d_\infty \quad . \tag{12}$$

Thus, the LE is proportional to the final distance between two nearby trajectories which is, in some cases, the variance of the velocity distribution. It is straightforward to demonstrate that α is given in units of the inverse length. In order to introduce a dimensionless parameter, we can scale α with a typical inverse length of the system $\rho^{1/3}$, where ρ is the density. Thus, the eq. (12) gives :

$$\hat{\lambda} = \alpha_0 \rho^{1/3} d_\infty \quad , \tag{13}$$

where α_0 is now a dimensionless constant. The results of eqs. (12), (13) are simple and rather transparent: the LE are given by the distances (variances) which provide a measure of the fluctuations. This is a very useful result which allows to estimate the LE using the final distributions obtained either from the data or from the theory such as the thermodynamics. For example, for a classical Boltzmann gas the variance of the distribution is given by [5] :

$$\sigma = \left(\frac{3T}{m}\right)^{1/2} \quad , \tag{14}$$

where T is the temperature of the gas and m the mass of the particles. In the ergodic limit, $\sigma = d_\infty$, thus the LE are obtained by substituting (14) in (13).

We have tested eqs. (9) - (14) using the MD approach. N particles interacting through a repulsive Yukawa potential have been randomly distributed in a large box with periodic boundary conditions at a temperature T. For each T, two trajectories differing initially by d_0 have been generated and $d(t)$ has been calculated at each time step t according to eq. (2). We have tested that the values of $\hat{\lambda}$ are independent of the choice of parameters a , b in (2) . Thus, in the following we set $a = 0$ and $b = 1$, i.e. we consider the distances in the velocity (or momentum) space only. In Fig. 1 we plot $d(t)$ vs. time for different values of d_0 for a fixed density and temperature. We see from the figure that all curves behave exponentially and we can deduce $\hat{\lambda}$ from a simple fit. Furthermore, the saturation value of $d(t)$ and the actual value of $\gamma = \hat{\lambda}$ are consistent with (9) and (10). Note that there are indeed some oscillations in the relative distance vs. time, but the oscillatory part is quite small and can be safely ignored, as we have done. The dependence of $\hat{\lambda}$ on the temperature for a Boltzmann gas is plotted in the upper part of Fig. 2. The solid line shows the fit with a $T^{1/2}$- dependence suggested by (14) .

Let us now define the normalized Lyapunov exponent (NLE) as:

$$\hat{\lambda}_N = \frac{\hat{\lambda}}{T^{1/2}\rho^{1/3}} \quad . \tag{15}$$

If (13) is correct, then NLE are constant and equal $\alpha_0(3/m)^{1/2}$. In the lower part of Fig. 2, we plot $\hat{\lambda}_N$ versus temperature T obtained in a MD simulation of a Boltzmann gas (open symbols). The calculations were performed for two densities: 0.01 fm^{-3} (open rombs) and 0.07 fm^{-3} (open squares). We can see that the NLE are constant within the error bars (for an explanation of the other symbol see below) and the value of α_0 equals approximately 1.

This result is quite instructive as it also tells us that any classical system interacting through the N-body potential should have the LE compatible with (14) and (15) in the limit of low density and high temperature, i.e. in the limit of an ideal gas. Therefore, to see deviations from the ideal gas limit it is quite useful to plot the NLE as defined in (15). Note also that one could generalize this finding to an ideal gas of fermions or bosons , since also in that case the variance in velocity space is known [5].

As a second example, let us estimate the LE using eq. (15) for a system undergoing a second order phase transition. We will discuss the case of a Bose-Einstein condensation near the so-called λ-point. The variance in velocity space for the superfluid part can be estimated from the scaling hypothesis [6] :

$$\sigma_s \propto \frac{1}{r_c} \propto (T_\lambda - T)^\nu \quad , \tag{16}$$

where r_c is the correlation length, T is the temperature and ν is a critical index. The index λ stands for the λ-point. The superfluid density ρ_s can be calculated in a similar manner :

$$\rho_s \propto (T_\lambda - T)^{(2-\alpha)/3} \quad , \tag{17}$$

where α is another critical index [5]. Inserting (16) and (17) into eq. (13) gives the LE :

$$\hat{\lambda} \propto (T_\lambda - T)^{(2-\alpha)/9+\nu} \quad . \tag{18}$$

A dynamical, microscopic model of the Bose-Einstein condensation is not available, so we cannot test (18) directly. But we can exploit an analogy with the system undergoing another second order phase transition, namely the liquid-gas phase transition. For that purpose , we will calculate the LE in MD using the interaction which consist of attractive and repulsive parts and exibits a liquid- gas phase transition at $T_c = 2.53\ MeV$ and $\rho_c = 0.04\ fm^{-3}$ [7] . The EOS for such interaction has been studied in ref. [7] and we will use the same numerical method discussed there for calculating the LE. Of course, we expect that at large T, since the density is rather low, the system should approach the ideal gas result. Thus we calculate the NLE as above. Using the scaling ansatz again we expect $hat\lambda_N \propto (T_c - T)^{\nu-1/2}$. In bottom part of Fig. 2, we plot the results obtained for this interaction (full squares). Note that at high T the results approach the ideal Boltzmann gas case as expected. For very low T, i.e. when the system is inside the instability region, the NLE are larger and have a maximum at the lowest calculated T in agreement with eqs. (15), (16). Unfortunately, because of numerical uncertainties in the estimation of the LE we cannot extract the value of the critical exponent but we notice that the accepted value of $\nu = 0.6 - 0.7$ obtained experimentally for a system undergoing a second order phase transition [5] , is compatible with our numerical results. We have tested our findings presented in Fig. 2 also by explicitly calculating the variances. The results are in good agreement with our predictions and we have not shown them in the figure to avoid the use of too many symbols.

Recently, Nayak et al. [8] have calculated the LE for a classical system undergoing a solid to liquid phase transition. These authors demonstrate that the LE dramatically increase at the melting point (see Fig.2 in ref. [8]). According to our findings the LE are proportional to the velocity variance. Again in ref. [8] it was found that the kinetic energy of the system has a dramatic change at the melting point as well. From Fig. 1 of ref. [8] one can easily see that the variance in the velocity also jumps as the cluster melts, which is a further proof of eq. (12). Of course, it would be interesting to reanalyze results of ref. [8] more quantitatively in the spirit of our approach.

In conclusion, in this paper we have found a relation between the Lyapunov exponents and the variance of the velocity distribution using the Navier-Stokes equation. Since this equation applies also to systems out of equilibrium, we expect our results to be valid for all cases where such an equation applies. In particular, our results are valid for systems in equilibrium for which we can derive analytical expressions for the LE. We have demonstrated the validity of our scheme using classical MD for a Boltzmann gas and for a liquid to gas phase transition [7] . We have also shown that the proportionality between the LE and the variances are consistent with the results of other authors regarding a solid to liquid phase transition [8]. We predict that LE have a power law dependence on T for systems undergoing a second order phase transition as in Bose-Einstein condensation and perhaps a transition to a quark gluon plasma. In the latter case, a measurement of hadron momenta in a 4π detector on an event by event basis should allow to determine the variances for each given hadron multiplicity. A plot of variances vs. multiplicity should show a power law behavior near the critical point (if the transition occurs). Similar considerations apply also to the liquid-gas phase transition predicted for nuclear matter and actively searched for in experiments involving heavy ion collisions [9] . Experimentally, one can obtain the Lyapunov exponents from the measured final velocity distribution of particles. From the equivalence demonstrated here of time averages with ensemble averages we expect that some relation can be found for other quantities like for instance the maximal LE and the Kolmogorov-Sinai entropy.

Acknowledgements

Two of us (A.B. and V.L.) thank the physics group of GANIL for warm hospitality and financial support. V.L. also thanks the Fondazione A. Della Riccia for a scholarship. We thank dr.A. Rapisarda for stimulating discussions.

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[1] For instance, the logistic map has been applied to the rate of reproduction of insects [2] as well as to an atomic nucleus undergoing evaporation [3]. More examples can be found in refs. [2] .

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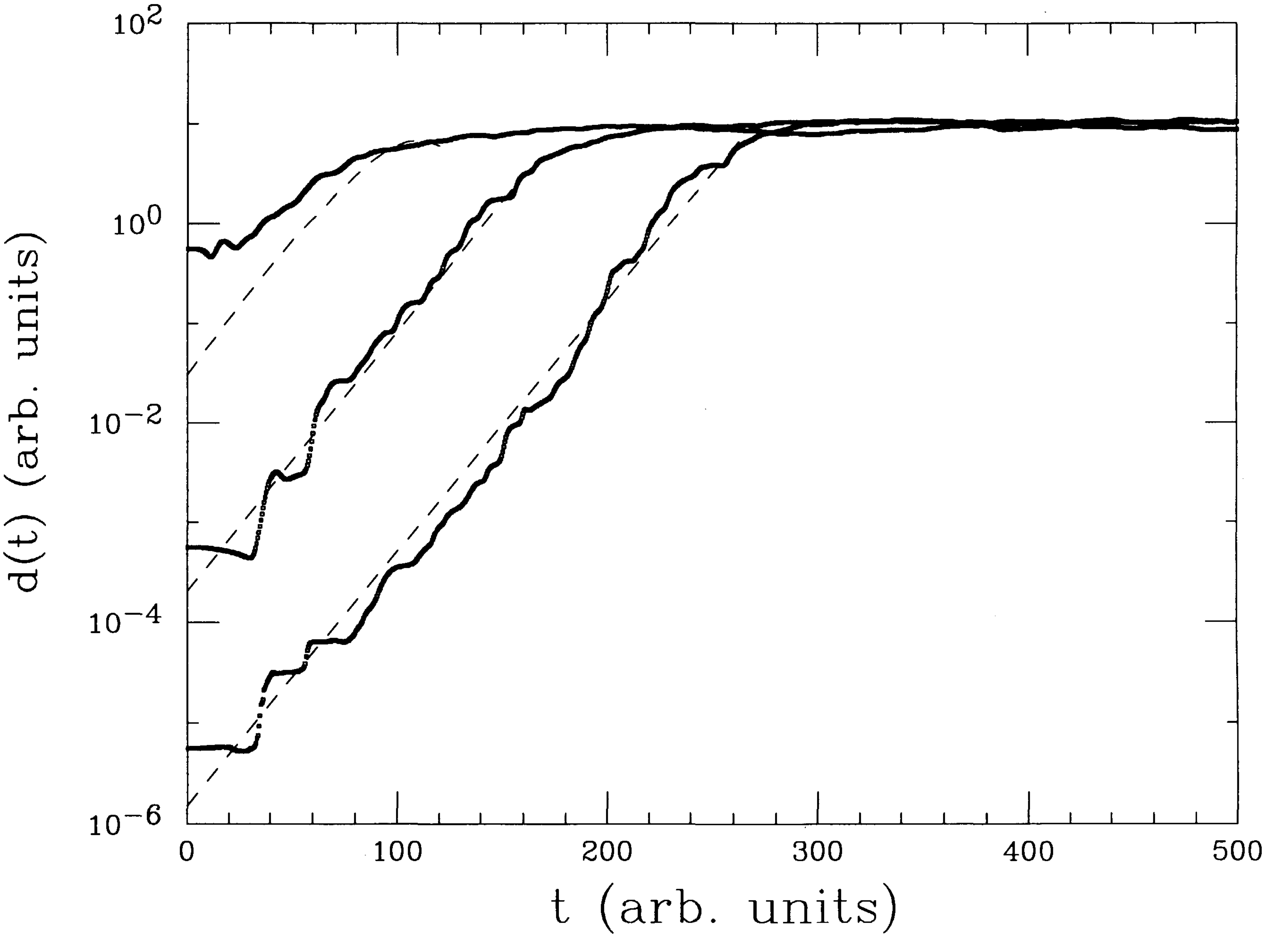
FIGURES

FIG. 1. Distance in momentum space vs. time for two trajectories which are calculated in classical MD for a fixed density and temperature. The initial distance d_0 was changed and three results are displayed. The dashed lines give a fit according to eqs. (9), (10).

FIG. 2. **(i)** Upper panel: The Lyapunov exponents (3), calculated using classical MD for a Boltzmann gas at various temperatures and for a fixed density, are plotted together with the $T^{1/2}$-fit (the solid line) suggested by (14). For details of the calculations, see the description in the text. **(ii)** Lower panel: Normalized Lyapunov exponents (15) vs. temperature for a classical Boltzmann gas at two different densities 0.01 fm^{-3} (open rombs) and 0.07 fm^{-3} (open squares). Full symbols depict the normalized Lyapunov exponents for a system at the critical density for a liquid-gas phase transition (0.04 fm^{-3}). The critical temperature for this system is $T = 2.53 MeV$.



10^2
10^0
10^{-2}
10^{-4}
10^{-6}
d(t) (arb. units)
0
100
200
300
400
500
t (arb. units)

Fig. 1

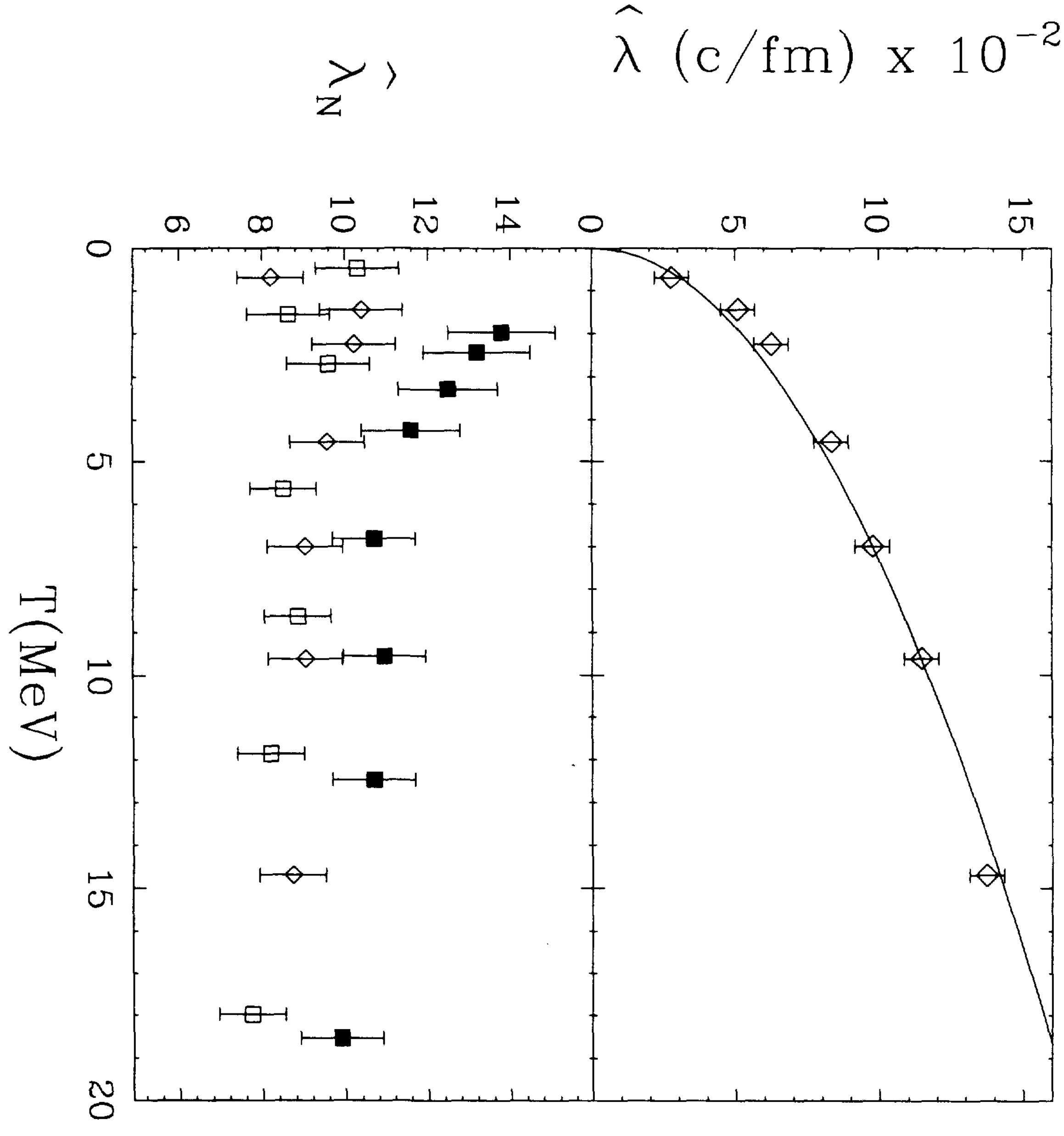


Fig. 2