Universal Behavior of Lyapunov Exponents in Unstable Systems

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We calculate the Lyapunov exponents in a classical molecular dynamics framework. Yukawa and Slater-Kirkwood forces are considered in order to give an equation of state that resembles the nuclear and the atomic ^{4}He equation of state, respectively, near the critical point for liquid-gas phase transition. The largest Lyapunov exponents λ are always positive and can be very well fitted near the "critical temperature" with a functional form $\lambda \propto |T - T_c|^{-\omega}$, where the exponent $\omega = 0.15$ is independent of the system and mass number. At smaller temperatures we find that $\lambda \propto T^{0.4498}$, a universal behavior characteristic of an order to chaos transition.

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The phenomena of phase transitions have been always a subject of great interest for many (generations of) physicists. Very recently there has been a large interest in studying what happens when the system is not composed of 10^{23} particles and confined in a box but, on the contrary, is composed of few hundred particles that are not confined. This interest was born first in heavy ion collisions where one would like to study the nuclear equation of state (NEOS) [1]. In the nuclear case it is not possible to study the infinite number of particles case (apart in stars, with the obvious difficulties), so one feasible way is to perform proton-nucleus or nucleus-nucleus collisions. In this manner it is possible to heat up and to explore different densities of the nuclei. Of course the problem is complicated apart from the fact of having a small number of particles, also from the presence of Coulomb force, angular momentum, and from the approximate knowledge of the "thermodynamical parameters," i.e., temperature, density, and pressure [2–4]. Similar problems can be found in the study of metallic clusters and/or fullerenes [5]. One of the first questions that arises is: Does it make sense to speak about phase transitions for a system made of 100–400 particles? To answer this question the authors of Refs. [3,5] and [6] have solved the exact classical many body problem [classical molecular dynamics (CMD)] numerically for particles interacting through two body forces. In particular, by preparing 100 particles in the ground state and giving to the particles an excitation energy (or temperature T) the following results are found:

(1) For a given initial temperature T_c the system undergoes multifragmentation [3,6,7]. The resulting mass distributions display a power law $Y(A) \propto A^{-\tau}$ with $\tau = 2.23$, which is exactly the value predicted in the Fisher droplet model for a system near the liquid-gas phase transition point [8]. Other critical exponents have also been estimated within the same model [7]: $\gamma = 0.86$, $\beta = 0.33$ [9]. Similar estimates but for experimental data on Au + C collisions at 1 GeV/nucleon [4] also give reasonable values of all the exponents.

(2) At the same temperature, fluctuations in the mass distribution are maximum. This is revealed through the study on an event by event analysis of intermittency signal, factorial moments, and Campi's plots [6,10,11].

(3) The "critical temperature" follows the scaling law $T_c/|E_b| = \text{const}$ [5], where E_b is the binding energy of the system (10.5 MeV for nuclei, 9.5 eV for C_{60} fullerenes, and 50.5 K for ^{4}He molecules).

(4) At very small temperatures or, equivalently, small excitation energies, the events are typical evaporationlike events, i.e., with a final mass distribution composed of a big fragment and many small ones: monomers, dimers, etc.

For some initial conditions the system displays large fluctuations; thus we expect that other indicators of fluctuations—the Lyapunov exponents—should be positive. The values of the Lyapunov exponents for systems undergoing a phase transition are not known (yet). In particular, the relationship between thermodynamical and dynamical properties has not been exhaustively explored. Ours is the first estimate of the Lyapunov exponents for systems exhibiting a critical behavior (possibly because of a liquid-gas phase transition). In a previous exploratory work, except for a two dimensional system and in the mean-field approximation, the largest Lyapunov exponents were calculated in the spinodal region [12]. It is well known, however, that the mean-field approximation gives a rough estimate of the critical exponents [8]; thus it is interesting to estimate their values in CMD.

We can summarize the main results of this work as follows: Independent of the studied system, i.e., nuclei, helium molecules, the largest Lyapunov exponents satisfy, similar to the Landau theory of phase transitions, the relation

$$\lambda = C|T - T_c|^{-\omega}, \qquad T \sim T_c\,, \tag{1}$$

where $\omega = 0.15 \pm 0.04$ and C is a constant.

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At smaller temperatures the Lyapunov exponents scale as

$$\lambda \propto T^{\ln 2/\ln \delta}, \tag{2}$$

with $\delta = 4.669\ldots$ the Feigenbaum constant [13] which indicates a typical transition from order to chaos [14,15].

Our studies are based on direct numerical simulation of an expanding system in classical molecular dynamics. In particular, we have studied a "nuclear" system where "neutrons" and "protons" interact through Yukawa potentials. Details of these forces can be found in Refs. [3,16]. The parameters entering the potentials have been fitted in such a way to have a ground state density of 0.16 fm^{-3}, a binding energy of -16 MeV/nucleon for an infinite system. For finite systems the binding energy is -10.5 MeV/nucleon without Coulomb forces. In this work we will discuss the parameter set that gives a soft EOS, i.e., compressibility $K = 250$ MeV [16] and the Coulomb interaction will be neglected. We notice that the use of the set corresponding to a stiff EOS, $K = 380$ MeV, gives the same results.

We have also studied He atoms interacting through the potential [17]

$$v(r) = 5.67 \times 10^6 e^{-21.5(r/\sigma)} - 1.08\left(\frac{\sigma}{r}\right)^6, \tag{3}$$

where $\sigma = 4.64$ Å and $v(r)$ is in kelvin.

Clearly the systems we are treating are quantal ones. However, we expect that a classical picture should give a reasonable description of the dynamics at high temperatures, i.e., near and above the critical temperature, since in these cases the densities reached are rather low with still high enough excitation energies. This is also demonstrated by the nice agreement of our CMD approach with data resulting from heavy ion collisions [3,6,7,16]. At very low temperatures quantum features become very important. Thus one should keep in mind that quantum fluctuations will change this scenario especially for $T \to 0$. In any case, it is very important to know the classical behavior of a quantum system since the quantal analog is reminiscent of classical chaos [15]. Unfortunately a fully microscopic treatment of quantum dynamics and fluctuations is still lacking.

In order to calculate the largest Lyapunov exponents [15] we first define the following metric in phase space:

$$d(t) = \sqrt{\sum_{i=1}^{N} [\alpha(\mathbf{r}_1'(t) - \mathbf{r}_2'(t))^2 + \beta(\mathbf{p}_1'(t) - \mathbf{p}_2'(t))^2]_i}\,, \tag{4}$$

where the sum runs over all the N particles of the system, the subscripts 1 and 2 refer to two events that at time $t = 0$ differ of an infinitesimal quantity $d(0) = 10^{-6}$ or less. The $\mathbf{r}'$ and $\mathbf{p}'$ are scaled positions and momenta. In our case

$$\mathbf{r}'(t) = \mathbf{r}(t)/R_{\mathrm{rms}}\,, \tag{5}$$

$$\mathbf{p}'(t) = \mathbf{p}(t)/P\,, \tag{6}$$

where R_{rms} is the root mean square radius and $P = \sqrt{2mT}$ is an average momentum, with m the nucleon (or the atom) mass and T the initial temperature (see below). Normally the Lyapunov exponents are calculated for systems bound in phase space. This is not always the case in our simulations since for high excitation energy the phase space explodes. In order to be certain of the soundness of our results we calculated the metric for three cases: (1) $\alpha = 1$ and $\beta = 1$, (2) $\alpha = 1$ and $\beta = 0$, (3) $\alpha = 0$ and $\beta = 1$. The results are independent of the choice of the metric, cases [1–3], as it should be.

The Lyapunov exponents λ are obtained from the relation

$$d(t) = d(0)e^{\lambda t}. \tag{7}$$

In our numerical simulations we prepared a system of 100 particles in their ground state. Then we distributed the moments of the particles according to a Maxwell-Boltzmann distribution at temperature T and let the system evolve in time by solving the classical equations of motion. At each temperature 100 events were generated. For each event (test event) ten other events were generated, each event differing from the test event of $d(0)$. The exponents were obtained by averaging over all the events. In order to get λ numerically, we calculated the ratio $d(t)/d(0)$ and fitted its exponential growth. As a check we estimated also

$$\dot{d}(t)/d(t) = \lambda\,. \tag{8}$$

In Fig. 1 we plot typical evolutions of $d(t)/d(0)$ at three temperatures $T = 2$, 5, and 20 MeV for the nuclear system. We see that the distance increases exponentially with time and can be very well fitted with a straight line (in a semilogarithmic plot) whose slope is just the Lyapunov exponent. The same results are found by using Eq. (8). In general we get Lyapunov exponents which are

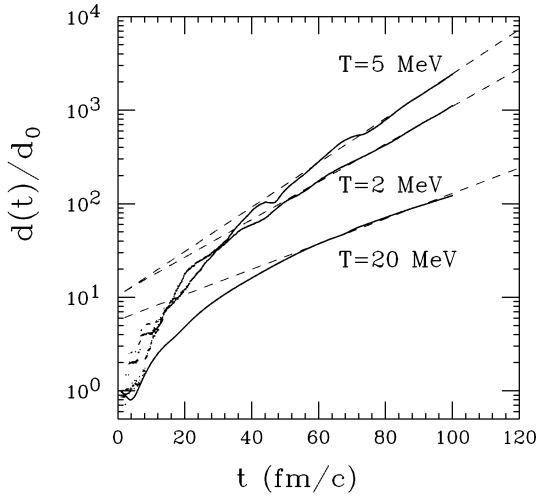

FIG. 1. The ratio $d(t)/d(0)$ is plotted as a function of time at three initial temperatures $T = 2$, 5, 20 MeV for the nuclear system. The dashed lines are fits whose slope give the typical λ for these temperatures after averaging over hundreds of events.

always positive at all temperatures and have a maximum value at $T \sim 4.5$ MeV. Similar behavior is found for the atomic case with a maximum at $T \sim 21.8$ K. In order to compare such different systems like nuclei or atomic He, we scale temperatures and times with typical values of the different systems. Usually one scales with the values obtained at the critical point. Since we do not know these values *a priori,* we scale the temperature with the absolute value of the binding energy and the (inverse) times with a typical value λ_0

$$\lambda_0 = \sqrt{2|E_b|/m}/R_0 . \tag{9}$$

Recall that in order to derive the EOS [8] one needs to know the hard core radius and the depth of the two body potential. These quantities are proportional to the average equilibrium distance between particles $R_0 = R/A^{1/3}$, where R is the radius of the system and A the mass number, and to the binding energy. In our case $\lambda_0 = 8.82 \times 10^{-5} \alpha c/a_0$ for the atomic one, with α the fine structure constant, c the speed of light, and a_0 the Bohr radius.

In Fig. 2 we plot the Lyapunov exponents at each initial temperature (in units of their typical values) for the nuclear (circle symbols) and atomic cases (squares). Note that the maximum value of λ is obtained at the initial scaled temperature

$$T_c/|E_b| \sim 0.43 \tag{10}$$

for both systems. For such temperatures the systems undergo multifragmentation and a power law in the mass distribution and factorial moments is found [3,6]. Thus our result confirms that in this temperature region fluctuations are largest. Inspired by the Landau theory of phase transition, we parametrized the exponents according to Eq. (1). The fit is also displayed in Fig. 2 (full and dashed curves). The same value $\omega = 0.15 \pm 0.04$ was used in both cases. We have obtained such a value by fitting the nuclear data with the functional form (1) and using C, T_c, and ω as free parameters, but imposing T_c larger than 0.4. Then we fixed the values of T_c and ω and fit C to the atomic data. By doing the same procedure but in reverse we get the error bar for ω.

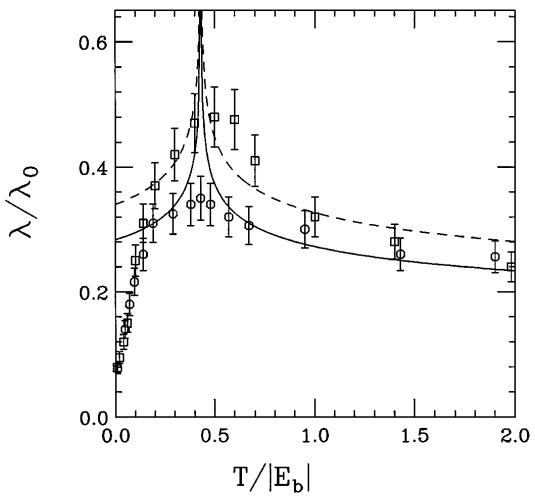

FIG. 2. The scaled largest Lyapunov exponents λ/λ_0 are plotted vs the scaled initial temperature $T/|E_b|$ for the nuclear (circles) and the atomic (squares) case. The full and dashed lines are fits obtained with the functional form $C|T - T_c|^{-\omega}$ where $\omega = 0.15 \pm 0.04$. The parameters of the fits are $C = 0.25$ and 0.3 for the nuclear and atomic cases, respectively. See text for further details.

Note the good agreement with the scaled λ at all temperatures but the lowest ones. For such small temperatures there is not any multifragmentation of the system, indeed the mass distribution reveals a typical case of evaporation. Using the same language as in the theory of phase transitions we could say that the small temperature cases explore densities and pressures outside the spinodal region. Note that the absolute values of the scaled exponents differ less than 30% for the two cases. Correspondingly the two fits differs only for a multiplicative constant C. The reason for such a small discrepancy is due to the fact that in the nuclear case we have two fluids, neutrons and protons. We will discuss this point in more detail in a following publication [18]. We also stress that these results are independent on the chosen metric, i.e., in the values of α and β in Eq. (4). We have also tested the results by changing the mass of the fragmenting system. The Lyapunov exponents remained the same for masses ranging from 50 to 400 particles [18]. The uncertainties reported in Fig. 2 are of the order of $\sim$10%.

A scaling law of Lyapunov exponents of the kind

$$\lambda \propto (A - A^*)^{\ln 2/\ln \delta} = (A - A^*)^{0.4498}, \tag{11}$$

where A is a control parameter and $\delta = 4.669\ldots$ the Feigenbaum constant [13], is typical of order to chaos transitions. The value A^* is the critical value which indicates the onset of chaos. Expression (11) was initially found in the logistic map [14], but various experiments have confirmed its general validity [15]. In our case the largest Lyapunov exponents λ are positive for all finite temperatures, i.e., the dynamics is always chaotic, but they tend to zero as the temperature T goes to zero. Actually for $T = 0$ the systems are frozen in their ground state and λ vanishes. Thus chaos starts at $T > 0$.

In Fig. 3 we plot a magnification of Fig. 2 for very small temperatures. The full curve is the expression (11) multiplied by a constant fitted on the numerical points. In this case the control parameter is the scaled temperature and A^* corresponds to $T = 0$. Agreement is impressive for both systems up to $T/|E_b| \sim 0.1$ [19].

Thus we have two different mechanisms at play. The first one for small temperatures gives a transition from order (the ground state) to chaos and has a dynamical origin. The second mechanism, for reduced temperatures larger than 0.1 has a thermodynamical origin appropriate for a second order phase transition. Loosely speaking, we have given evidence for "critical chaos" in the latter case.

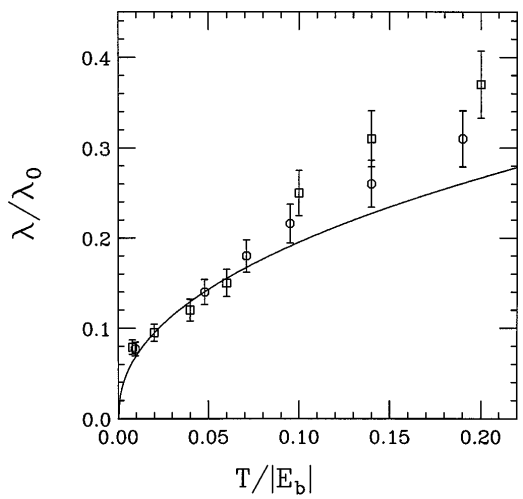

FIG. 3. A magnification of Fig. 2 at very small temperatures. The full curve is a fit with the functional form $KT^{0.4498}$ where $K = 0.55$ is the fitted parameter. See text for further details.

In conclusion, in this work we have calculated the largest Lyapunov exponents as a function of the initial temperature for an expanding system composed by 100 particles in the framework of classical molecular dynamics. We have shown that these exponents are always positive and have their largest value at a temperature of $\sim$0.45 MeV for the nuclear case and $\sim$21.8 K for the atomic one. We have also demonstrated that the λ obey universal scaling laws. They fulfill the relation $|T - T_c|^{-\omega}$, $\omega = 0.15 \pm 0.04$, similar to the Landau theory of phase transitions near the critical point. At the same time, for smaller temperatures (evaporation events) Lyapunov exponents exhibit a general transition from order ($T = 0$) to chaos ($T > 0$). We feel that further investigations following the ideas presented in this Letter may help our understanding of order and disorder in classical systems and, after all, in (part of) nature itself.

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[19] Note that if we fit the data points of Fig. 3 with the functional form $y = ax^b$, a and b being the fitting parameters, we get $a = 0.87(0.01)$, $b = 0.53(0.06)$ including the values up to $T/|E_b| = 0.1$, while we obtain $a = 0.50(0.08)$ and $b = 0.41(0.05)$ if we fit up to $T/|E_b| = 0.75$. Clearly the low energy region we are interested in is up to 0.1, where the results for atomic and nuclear case start to differ and a different regime sets in. Thus the actual value used in Fig. 3, $b \sim 0.45$, which seems to be a universal number for a general order-to-chaos transition [14,15], is compatible with the values obtained through the fits.