Lyapunov exponents in unstable systems

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We investigate the dynamical behavior of unstable systems in the vicinity of the critical point associated with a liquid-gas phase transition. By considering a mean-field treatment, we first perform a linear analysis and discuss the instability growth times. Then, coming to complete Vlasov simulations, we investigate the role of nonlinear effects and calculate the Lyapunov exponents. As a main result, we find that near the critical point, the Lyapunov exponents exhibit a power-law behavior, with a critical exponent $\beta=0.5$. This suggests that in thermodynamical systems the Lyapunov exponent behaves as an order parameter to signal the transition from the liquid to the gas phase. [S1063-651X(99)09107-2]

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I. INTRODUCTION

In recent years the study of liquid-gas phase transitions has been the object of a renewed interest in different fields of physics, expecially because of the possible connection to the description of the disassembly of systems out of equilibrium [1–3]. In particular, second-order phase transitions are known to exhibit general thermodynamical properties, which are common to different complex systems. For instance, the so-called critical exponents, which characterize the behavior of various physical observables (such as the fluctuation correlation length) nearby the critical points of the phase diagram under consideration, have been largely studied [4].

While the statistical properties of systems presenting a coexistence of two or more phases seem now well established, the dynamical properties and the time scales involved in the phase-transition process are presently under investigation [2,3,5,6]. In the case of systems unstable against density fluctuations (such as systems undergoing a liquid-gas phase transition), the dynamical evolution is dominated by the exponential growth of the local density perturbations. This means also that two different trajectories, having a small initial relative distance d_0 in phase space, will soon diverge exponentially. From this point of view, the Lyapunov exponents [7] appear as an appropriate observable to study in order to extract information on the dynamical evolution of the system, since they tell how much two nearby trajectories are separated after a time t.

In situations exhibiting a chaotic behavior, such as, for instance, the case of the logistic map [7], the Lyapunov exponents λ are known to signal the transition from order ($\lambda<0$) to chaos ($\lambda>0$). In the vicinity of a ''critical point'' r_c, λ becomes equal to zero and, hence, it can be seen as an order parameter that indicates the onset of chaos. The analogy with critical phenomena can be pushed further by writing $\lambda\propto(r-r_c)^\beta$, where β can be interpreted as a critical exponent. Following this analogy, it is interesting to show that also in thermodynamical systems the Lyapunov exponent behaves as an order parameter in the vicinity of a critical point.

We will work out a numerical estimation of Lyapunov exponents, in the mean-field approximation, for a system located near the critical point associated with a liquid-gas phase transition, and we will try to discuss some general features, not depending on the nature of the system considered. In particular, we will show that, at the critical density ρ_c, the largest Lyapunov exponent vanishes as $(1-T/T_c)^\beta$, where T_c is the critical temperature, with $\beta\approx0.5$. Preliminary calculations have been performed using classical molecular-dynamics simulations of a system exhibiting a liquid to gas phase transition [6]. In that case it was, however, numerically difficult to extract the behavior of λ in terms of critical exponents.

II. MEAN-FIELD DESCRIPTION OF UNSTABLE SYSTEMS

We will perform this study in the framework of a mean-field approach. Let us consider, for the sake of simplicity, the case of an infinite medium of particles having mass m. The time evolution of the one-body density function $f(\mathbf{r},\mathbf{p},t)$ is governed by the Vlasov equation, which is written below:

$$\frac{\partial f}{\partial t}+\frac{\mathbf{p}}{m}\cdot\frac{\partial f}{\partial \mathbf{r}}-\frac{\partial U[f]}{\partial \mathbf{r}}\cdot\frac{\partial f}{\partial \mathbf{p}}=0, \tag{1}$$

where $U[f]$ denotes the self-consistent mean-field potential. For instance, one could consider a Skyrme-like parameterization: $U(\rho)=\frac{3}{4}t_0\rho+\frac{3}{16}t_3\rho^2$ [8], where $\rho(\mathbf{r},t)$ is the spatial density: $\rho(\mathbf{r},t)=\int d\mathbf{p}f(\mathbf{r},\mathbf{p},t)$. The parameters t_0,t_3 can be adjusted in order to reproduce saturation properties (such as saturation density and binding energy) of the system considered.

III. LINEAR ANALYSIS OF UNSTABLE SYSTEMS

Important information about the dynamical evolution of an unstable system can be obtained already by performing a linear-response analysis. This allows us to investigate the early growth of instabilities and to calculate the instability growth times. It is of interest to compare the inverse of the growth times, which signal the occurrence of instabilities, with the Lyapunov exponents that are sensitive to nonlinear effects. A complete solution of the Vlasov equation will be considered in the next chapter. Then, since nonlinear effects will also be present, we will calculate the Lyapunov exponents and discuss the role of chaos.

The small fluctuations δf around a thermal equilibrium identified by f_0 are determined considering the linearized equation:

$$\frac{\partial \delta f}{\partial t}+\frac{\partial \delta f}{\partial \mathbf{r}}\cdot\frac{\mathbf{p}}{m}-\frac{\partial f_0}{\partial \mathbf{p}}\cdot\frac{\partial \delta U}{\partial \mathbf{r}}=0, \quad (2)$$

where δU represents the fluctuating part of the mean-field potential. Carrying out a Fourier transform with respect to time and considering the plane-wave representation, we obtain the following dispersion relation for the frequency ω_k of the collective mode associated with the wave number k [9]:

$$1=\int d\mathbf{p}\left(\frac{\partial U_k}{\partial \rho}\frac{\mathbf{p}\cdot\mathbf{k}}{m}\frac{\partial f_0}{\partial \epsilon}\right)\Bigg/\left(\omega_k+\frac{\mathbf{p}\cdot\mathbf{k}}{m}\right), \quad (3)$$

where $\epsilon=\mathbf{p}^2/(2m)$, and U_k is the Fourier transform of the mean-field potential. The solutions ω_k come by pairs of opposite sign, similarly as we will see later on to the λ. It turns out that for systems initialized inside an unstable region of their phase diagram (such as systems undergoing a liquid-gas phase transition), the solutions ω_k become imaginary, so that the local-density fluctuations are amplified, leading to an instability. It should be noticed that, in this situation and within the linear analysis, the divergence of two close trajectories is just due to the presence of instabilities, such as in the case of systems of uncoupled inverted (unstable) oscillators [10]. As a measure of the instabilities, we will consider the inverse of the characteristic growth time for the amplification of fluctuations : $-i\omega_k=1/\tau_k$.

Let us concentrate on the behavior of ω_k in the vicinity of the border of the unstable region (the spinodal border). All along this line ω_k is equal to zero and it is interesting to investigate how the solutions of Eq. (3) reach this limit. To perform this analysis, let us consider two examples: a gas of fermions ($f_0=\{1+\exp[(\epsilon-\mu)/T]\}^{-1}/h^3$) and a gas of classical particles $[f_0=\rho/(2\pi mT)^{3/2}\exp(-\epsilon/T)]$ initialized at a given temperature T and density ρ. μ denotes the chemical potential.

A. Fermionic systems

Let us first consider the case of fermions. At zero temperature, for imaginary frequencies, Eq. (3) can be rewritten under the form,

$$1+1/F_0(k)=\gamma_k \ \arctan(1/\gamma_k), \quad (4)$$

where $\gamma_k=-i\omega_k/(kv_F)$, and v_F is the Fermi velocity, analogous to the Lyapunov exponent. Here we have introduced the Landau parameter $F_0(k)=(3/2)(\partial U_k/\partial\rho)(\rho/\epsilon_F)$, as done in Ref. [9].

At finite temperature, an approximate solution to the dispersion relation (3) is obtained by considering the Sommerfeld expansion for f_0, truncated at the second order in (T/ϵ_F). Then Eq. (3) can be still approximately rewritten under the form (4) after introducing the temperature-dependent Landau parameter $F_0(k,T)=F_0(k,T=0)[1-\pi^2/12(T/\epsilon_F)^2]$. In order to study the behavior of γ_k near the critical point, let us expand the left hand side of Eq. (4) around the critical temperature T_c. Considering the expansion up to second-order terms, we have $1+1/F_0(k,T)=a_k(1-T/T_c)+1/2b_k(1-T/T_c)^2$, with $a_k=-F_0(k,T=0)(\pi^2/6)(T_c/\epsilon_F)^2$ and $b_k=-a_k-F_0^2(k,T=0)(\pi^4/18)(T_c/\epsilon_F)^4$. Now the dispersion relation can be solved considering that in the range of solutions of our interest, $\gamma_k\arctan(1/\gamma_k)\approx\pi/2\gamma_k-\gamma_k^2$. The solution is

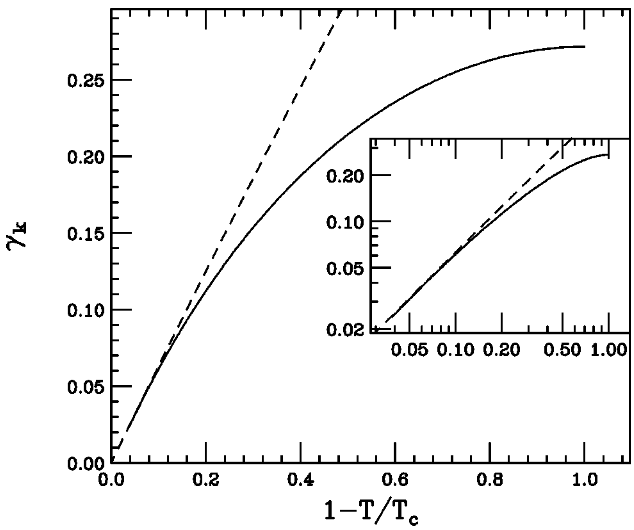

FIG. 1. The value of $\gamma_k=-i\omega_k/(kv_F)$ is plotted as a function of $(1-T/T_c)$ (solid line) in the case of a system of fermions. The dashed line represents the result obtained for a classical system. In the inset we plot the two curves on a log-log scale.

$$\gamma_k\approx\pi/4-\sqrt{\pi^2/16-[1+1/F_0(k,T)]}. \quad (5)$$

Developing up to second-order terms in $(1-T/T_c)$, we obtain:

$$\gamma_k\approx 2/\pi a_k(1-T/T_c)+1/2(16/\pi^3a_k^2+2/\pi b_k)(1-T/T_c)^2, \quad (6)$$

which shows that when $T\approx T_c$, the behavior of γ_k is linear.

The solution of the dispersion relation (3) is presented in Fig 1 (solid line). In the calculations we have taken $F_0(T=0)=-1.36$ and $\epsilon_F=19.5$ MeV. This corresponds to the density value $\rho=0.065$ fm^{-3} and $k=0.6$ fm^{-1}, which is the mode for which the largest value of γ_k is obtained (the most unstable mode). In the inset of Fig 1, the curve is plotted in a log-log scale.

B. Classical systems

In the case of classical systems, the dispersion relation (3) can be approximately solved considering again the solutions of Eq. (4), where $\gamma_k=-i\omega_k/(k\overline{v})$, and $\overline{v}$ is the average particle velocity associated with the temperature T:$\overline{v}=2/(m\pi)^{1/2}(2T)^{1/2}$, and with the Landau parameter $F_0(k,T)$ defined as $F_0(k,T)=(\partial U_k/\partial\rho)(\rho/T)$. Now the left-hand side of Eq. (4) can be written as follows: $1+1/F_0(k,T)=F_0(k,T_c)(T/T_c-1)=(1-T/T_c)$. We find

$$-i\omega_k\approx 2k(2T/m\pi)^{1/2}[\pi/4-\sqrt{\pi^2/16-(1-T/T_c)}]. \quad (7)$$

Developing up to second-order terms, the solution is

$$\gamma_k \approx 2/\pi(1-T/T_c) + 1/2(16/\pi^3 - 2/\pi)(1-T/T_c)^2. \quad (8)$$

The solution for γ_k is presented in Fig. 1 (dashed line).

As it is possible to see from the figure and also from the shape of the approximate solutions [Eqs.(6) and (8)], in the linear approximation, i.e., considering only the first-order terms in δf, the behavior of γ_k around the critical temperature is linear. Indeed, in the vicinity of T_c we find $\gamma_k \propto (1-T/T_c)$.

The same behavior is found not only around the critical point, but also all along the spinodal line.

IV. COMPLETE VLASOV SIMULATIONS

It should be noticed that in complete mean-field calculations also higher-order terms in δf will play a role, especially in the unstable region. Indeed, the complete Vlasov equation contains nonlinear terms, which are expected to become more and more important when approaching the spinodal border and the critical point. When nonlinear effects play an important role, chaos sets in and the behavior of the Lyapunov exponents λ can give important indications on this process. An evaluation of λ can be obtained by considering a numerical solution to the Vlasov equation. In this way all nonlinear effects will be taken into account. We solve the Vlasov equation using the test particle method: a given number of test particles N_{test} is associated with each particle of the system, i.e., we write

$$f(\mathbf{r},\mathbf{p},t) = \mathcal{C} \sum_i^{N_{test}\cdot A} g(\mathbf{r}-\mathbf{r_i}) g(\mathbf{p}-\mathbf{p_i}),$$

where the sum runs over the total number $N = N_{test}\cdot A$ of test particles (A is the number of particles) and the functions g are Gaussians. $\mathcal{C}$ is a normalization factor. Inserting this expression into the Vlasov equation [Eq. (2)] gives the equations of motion for the test particles:

$$\dot{\mathbf{r}}_i = \mathbf{p}_i/m; \quad \dot{\mathbf{p}}_i = -\nabla_i \langle U \rangle, \quad i=1,\dots,N.$$

Finally, from the time evolution of the test particles it is possible to trace back the time behavior of the one-body density function [8]. It should be noted that because of the random sampling of the phase space due to the use of a finite number of test particles, this method naturally introduces some fluctuations in the solution of the Vlasov equation.

We will present calculations performed for an infinite system of fermions, using periodic boundary conditions. In the case of classical systems, the same qualitative behavior is obtained.

We consider the density value $\rho_0 = 0.065 \ \mathrm{fm}^{-3}$ and several temperature values. $N = 10\,560$ test particles have been used, and 50 events, differing just because of the fluctuating initial conditions, have been considered. To keep the analogy with the previous discussion on the instability parameter γ_k, we have adopted the following definition of the Lyapunov exponent: $\lambda = (1/t)\ln[d(t)/d(0)]$, with

$$d^2(t) = \sum_r \delta\rho_r^2 = \sum_r (\rho_r - \rho_0)^2. \quad (9)$$

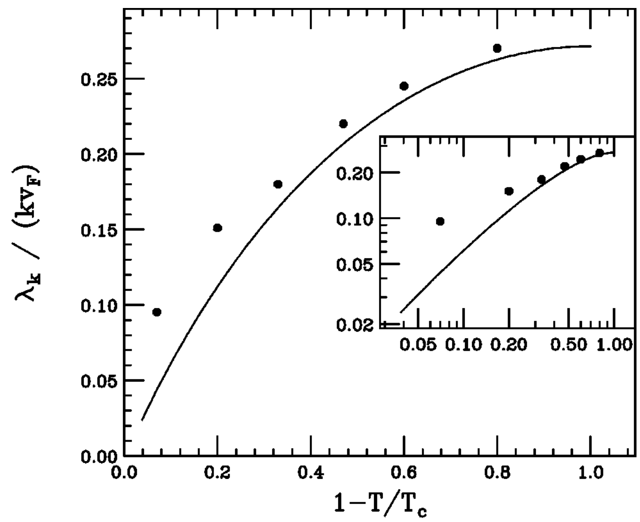

FIG. 2. The largest Lyapunov exponent $\lambda_k/(kv_F)$, obtained in the case of a fermionic system, is plotted as a function of $(1-T/T_c)$ (full circles). The value of γ_k is also reported for comparison (full line). In the inset the results are plotted on a log-log scale.

As in Ref. [5], the distance $d(t)$ is obtained dividing the space into cells and calculating the difference between the perturbed density ρ_r and ρ_0. The sum Σ_r runs over the sites of the space cells.

Then we consider the Fourier transform $\delta\rho_k(t)$ of the time-dependent density fluctuation $\delta\rho_r(t) = \rho_r(t) - \rho_0$, and we construct the equal time correlation function $\sigma_k^2(t) = \langle \delta\rho_k(t)\,\delta\rho_k(t)\rangle$ (where the ensemble average is taken over the 50 events considered). We define the k-dependent Lyapunov exponents as $\lambda_k(t) = 1/(t)\ln[\sigma_k(t)/\sigma_k(0)]$. The value of λ_k is taken at large times, when a plateau is observed in the time evolution. We notice that this definition allows us to study separately the behavior of the modes of the spatial density associated with the wave number k. So this can be considered as an analysis in terms of plane waves (or spectral analysis) of the Lyapunov exponent λ [Eq. (9)] [11]. In Fig. 2 we plot the value of $\lambda_k/(kv_F)$ (full circles) for the mode $k = 0.6 \ \mathrm{fm}^{-1}$ that gives the largest value of λ_k as a function of the temperature and we compare it to the trend observed in the same situation for γ_k (solid line). In this way one can investigate the role of nonlinear effects and the onset of chaos. In the inset the results are plotted in a log-log scale. We observe a discrepancy with respect to the behavior given by the linear response analysis, especially in the high-temperature region. In particular, it is possible to see that the behavior of the Lyapunov exponent around $T = T_c \approx 15 \ \mathrm{MeV}$ is not linear. The differences observed between λ_k and γ_k can be considered as an indication of the importance of nonlinear effects in complete Vlasov calculations.

We have considered also a different possible evaluation of the largest Lyapunov exponent. We will adopt the definition used in Ref. [12]: $\lambda = (1/t)\ln[d(t)/d(0)]$, with

$$d^2(t) = \sum_{i=1}^{N} [\alpha_r(\mathbf{r}_i^{(1)} - \mathbf{r}_i^{(2)})^2 + \alpha_p(\mathbf{p}_i^{(1)} - \mathbf{p}_i^{(2)})^2]/N. \quad (10)$$

$d(t)$ represents the distance in phase space between two

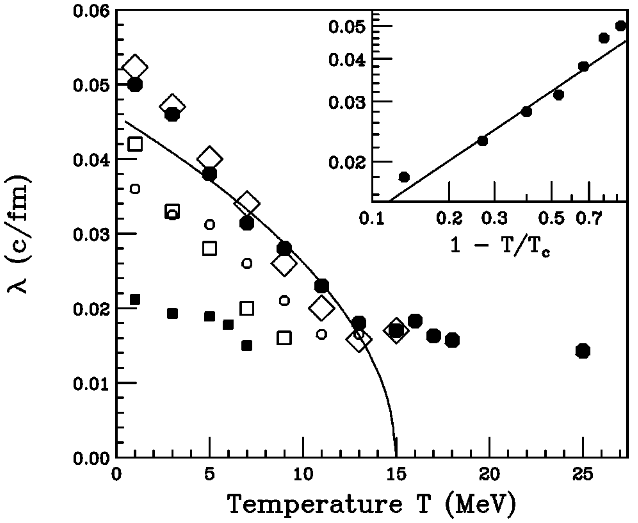

FIG. 3. The largest Lyapunov exponent λ (see text for detail) as a function of the temperature for different density values: diamonds, $\rho = 0.04\ \mathrm{fm}^{-3}$; full circles, $\rho = 0.06\ \mathrm{fm}^{-3}$; open squares, $\rho = 0.02\ \mathrm{fm}^{-3}$; open circles, $\rho = 0.08\ \mathrm{fm}^{-3}$; full squares, $\rho = 0.09\ \mathrm{fm}^{-3}$. The solid line represents a fit of the points obtained at $\rho = 0.06\ \mathrm{fm}^{-3}$. These points and the fit are plotted in a log-log scale in the inset.

close trajectories (1) and (2). As shown in Ref. [12], the results obtained for λ are independent of the values used for α_r and α_p.

Here we use $\alpha_r = 0, \alpha_p = 1$. Indeed, in a homogeneous infinite system, the resulting definition, based on the momentum distance among particles of close trajectories, is well suited to study the response of the system to a small initial perturbation. In fact, in absence of perturbations, since the system is perfectly homogeneous, the particles do not feel any force; the distance $d(t)$ would not evolve and λ would be zero.

In Fig. 3 the results are plotted at different density values as a function of the temperature. We note that the results are very similar to the ones obtained in the case of the largest λ_k (see Fig. 2). The important point to notice is that around the critical density $\rho_c \approx 0.06\ \mathrm{fm}^{-3}$, the behavior of λ as a function of the temperature is of the type $(1 - T/T_c)^\beta$, with $\beta = 0.5$. Indeed it is possible to fit the points with a curve $\lambda \propto (1 - T/T_c)^{0.5}$ (solid line). This result suggests that the Lyapunov exponent behaves as an order parameter nearby the critical point associated with a liquid-gas phase transition. Also, it is interesting to notice that according to the Landau theory, the critical exponent expected in the mean-field theory is equal to $\beta = 0.5$ [13]. Actually, in our numerical calculations the Lyapunov exponents are not zero along the spinodal line, but we observe a saturation around the value $\lambda = \lambda_{sat} \approx 0.015\ \mathrm{fm}^{-1}$. This is due to the use of a finite number of test particles in the simulations. In fact the finite mapping of the phase space creates some small fluctuations in the mean field and the particles move in response to that, even in stable situations, where these fluctuations are not amplified. Consequently, the Lyapunov exponent keeps a finite value. Going to the limit of an infinite number of test particles, the spatial density would become perfectly homogeneous. Hence, the particles would not see any variation of the mean-field potential and λ would vanish. Apart from this

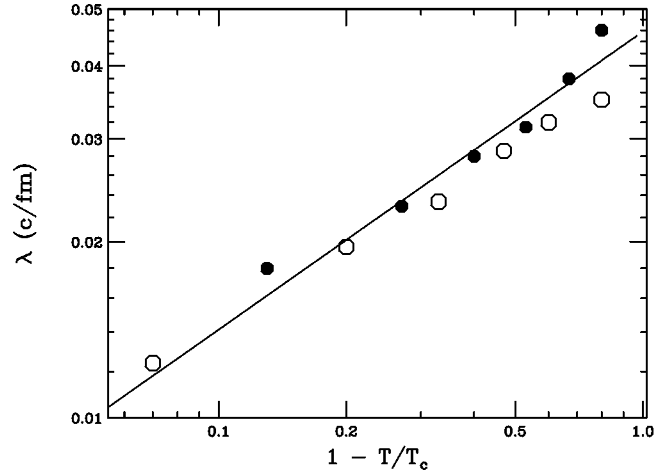

FIG. 4. The largest Lyapunov exponent λ (full circles) is compared to the largest λ_k (open circles), at the critical density $\rho \approx 0.06\ \mathrm{fm}^{-3}$. The solid line represents a fit with a power law.

saturation problem, the λ defined by Eq. (10) and the largest λ_k take quite similar values, as is shown in Fig. 4.

In conclusion, the introduction of nonlinear effects (and the possible occurrence of chaos) essentially determines a change of the exponent β. Indeed we have seen that in the linear approximation the inverse of the instability growth time γ vanishes linearly in the vicinity of the critical point.

In Fig. 5 we use a different representation and we plot, for different temperature values, the Lyapunov exponent as a function of the density. At the critical temperature, the Lyapunov exponent reaches its saturation value for all densities considered while reducing the temperature it increases, and reaches the maximum value in correspondence to densities close to the critical density.

V. CONCLUSIONS

We have investigated the behavior of thermodynamical systems located nearby the critical point associated with a liquid-gas phase transition. In the linear approximation, we

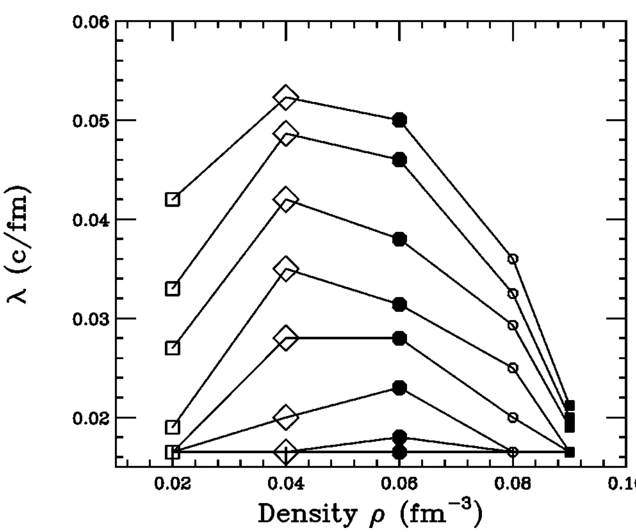

FIG. 5. The largest Lyapunov exponent λ as a function of the density. The different curves are isotherms. The temperature values are (from top to bottom) 1,3,5,7,9,11,13, and 15 MeV.

study the instability growth times. We find that the growth times vanish linearly ($\beta=1$) along the spinodal border, indicating the transition from unstable to stable situations. Solving numerically the complete Vlasov equation, we discuss the behavior of the Lyapunov exponents. This analysis indicates the importance of nonlinear effects that could signal the onset of chaos when the temperature approaches the critical temperature. The trend observed follows a power-law behavior: $\lambda \propto (1-T/T_c)^{\beta}$, with $\beta=0.5$. This suggests that the Lyapunov exponent can be seen as an order parameter to signal the transition from the liquid to the gas phase. The value found for the critical exponent $\beta=0.5$ is in agreement with the predictions of the Landau mean-field theory. Considering the case of classical and fermionic systems, we find that the value of the critical exponent is independent on the statistics of particles.

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