Slow relaxation and phase space properties of a conservative system with many degrees of freedom

S. Flach*
Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215

G. Mutschke
Research Center Rossendorf, P.O. Box 51 01 19, 01314 Dresden, Federal Republic of Germany
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The object of our study is the one-dimensional discrete Φ^4 model. We compare two equilibrium properties by use of molecular dynamics simulations: the Lyapunov spectrum and the time dependence of displacement-displacement and energy-energy correlation functions. Both properties imply the existence of a dynamical crossover of the system at the same temperature. This correlation holds for two rather different regimes of the system — the displacive and intermediate coupling regimes. These results imply a deep connection between slowing down of relaxations and phase space properties of complex systems.

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I. INTRODUCTION

The classical statistical mechanics of macroscopic systems in equilibrium essentially uses the ergodicity conjecture, i.e., time averages are replaced by phase space averages. The nongeneric occurrence of integrable systems and the existence of stochastic webs in the phase space of nonintegrable systems with $N \geq 3$ (N is the number of degrees of freedom) [1] together with Boltzmann's approach (cf., e.g., [2]) provides an intuitive explanation of the ergodicity conjecture. However the dynamics of nonlinear macroscopic systems shows up with rather complex properties so that further details of nonlinear dynamics have to be exploited. In this contribution we deal especially with properties of slow relaxations. Common examples could be critical slowing down near second order phase transitions [3] and freezing near the liquid-glass transition [4]. In these problems one has to deal with dynamics on different time scales. The success of phenomenological and semiphenomenological theories to describe slow relaxations in those systems does not alter the fact that we are far from completely understanding the underlying microscopic dynamics.

The modern theory of nonlinear dynamics provides us with several useful results. First we mention the Kolmogorov-Arnold-Moser theorem (KAM) [1]. It states that if an integrable system is slightly perturbed with a nonintegrable perturbation, there exists a set consisting of N-dimensional tori close to the tori of the unperturbed integrable system. The set in the perturbed system is nowhere dense but forms a large part of the phase space (i.e., the measure of the complement of the set tends to zero as the perturbation is lifted). If the perturbation strength overcomes a finite value, most of the perturbed tori are destroyed. The KAM theorem deals only with the possibility of a nonintegrable system to evolve on regular trajectories (tori). In that sense KAM makes no statements about finite time stabilities. Second we mention the Nekhoroshev theorems [5]. These theorems deal with finite time stabilities. They provide us with lower bounds on time scales on which the nonintegrable system evolves on a trajectory close to a regular one. Finally we mention the numerical evidence for the existence of strong stochasticity thresholds (SST) (in the strength of the perturbation) [6]. Below the SST the system's trajectory evolves mainly along resonances in phase space. Above the SST the trajectory evolves across resonances thus speeding up the relaxation of the system, which can be roughly brought into connection with the time the system's trajectory needs to cover a major part of the available phase space.

A subtle point in the application of the above results to macroscopic systems is the dependence of different threshold values on the number of degrees of freedom. Despite controversial opinions there seems to be some agreement that neither the KAM tori nor the Nekhoroshev finite time regularity survive in the limit $N \to \infty$ [7]. In other words, those properties are suppressed to regions of almost zero energies per degree of freedom (temperature) in the thermodynamic limit. Only the SST seems to survive. The increase of the energy per degree of freedom in a nonlinear nonintegrable system is equivalent to the increase of the strength of a certain nonintegrable perturbation. Then it could be possible that at certain finite energies per degree of freedom the system will be close to another integrable system. For instance it is possible for certain systems to increase the energy per degree of freedom to infinity and become infinitely close to an integrable system. Thus we would not *a priori* rule out the applicability of the KAM and Nekhoroshev results to macroscopic systems at finite temperature.

In this work we present results of numerical experiments for a simple one-dimensional lattice model. We show that both the relaxation times and Kolmogorov-Sinai entropy (KSE) are sensitive to the existence of a

*Electronic address: flach@buphy.bu.edu

dynamical "phase transition." In other words we can deduce changes in relaxational properties by measuring the KSE and changes in the type of phase space trajectories by measuring relaxation times. The interpretation of our results is (in our opinion) closely connected to the thresholds discussed in the above paragraph. It is also useful in detecting new kinds of elementary excitations (quasiparticles) in complex systems, as we will demonstrate by analyzing two particular model realizations.

II. MODEL, NUMERICAL METHODS

We study a $d = 1$ dimensional discrete classical model given by the Hamiltonian

$$H = \sum_{l=1}^{N} \left[\frac{1}{2} P_l^2 + \frac{1}{2} C (X_l - X_{l-1})^2 + V(X_l) \right] \quad . \tag{1}$$

P_l and X_l are the canonically conjugated momentum and displacement of the l th particle, where l marks the number of the unit cell. C measures the interaction to the nearest neighbor particles. All variables are dimensionless. The mass of the particles is equal to unity. N is the total number of particles. The nonlinearity appears in the "on-site" potential $V(x)$ which is of the Φ^4 type:

$$V(x) = V_{\Phi^4}(x) = \frac{1}{4}(x^2 - 1)^2 \quad . \tag{2}$$

The barrier height of this double well potential is $\Delta = 0.25$. The interaction parameter C and the energy per particle E/N (E is the total energy of the system) are the two parameters of the system. The temperature T (mean squared velocity) is then given through a virial theorem. The classification of the system behavior in the (C, T) plane turns out to be rather complex. First we mention the existence of a critical point (second order phase transition) on the line $(C, T_c = 0)$ [8]. The order parameter is $\langle X \rangle = \sum_l X_l$. For finite temperatures below the value of Δ one finds the following: Ising-like (order-disorder) behavior for $C \ll 1$, displacive (continuous) behavior for $C \geq 1$, and a subtle intermediate behavior in between the two previous C ranges. For temperatures tending to infinity the system behaves like uncoupled quartic oscillators with canonical energy distribution. For any finite value of C the correlation length ξ will decrease from infinity ($T = 0$) to zero ($T = \infty$). Fixing the temperature one finds zero correlation length for $C = 0$. Increasing C leads to an increase of ξ. For $C \to \infty$ the correlation length tends to infinity. This is due to the fact that the critical region around $T_c = 0$ increases as the interaction is increased.

The slow relaxational dynamics of our system is, in part, our focus. The simplest way to describe it would be to consider the correlation function $S_{A_l A_k}(\omega)$,

$$\begin{gathered} S_{A_l A_k}(t) = \langle A_l(t) A_k \rangle \ , \ S_{A_l A_k} = \langle A_l A_k \rangle \ , \\ S_{A_l A_k}(\omega) = i S_{A_l A_k}(z = \omega + i0) \ , \\ F(z) = \mathcal{L}[F(t)] = \frac{1}{i} \int_0^\infty dt e^{izt} F(t) \ . \end{gathered} \tag{3}$$

Here $\langle ... \rangle$ denotes the standard canonical average and $\mathcal{L}[...]$ means Laplace transformation. The local microscopic variable A_l could be any combination of the canonical variables setting up our desired Hamiltonian in (1) and (2). The imaginary part of the susceptibility is then defined as

$$\chi''_{A_l A_k}(\omega) = \omega S_{A_l A_k}(\omega) / S_{A_l A_k}(t = 0) \tag{4}$$

and can be studied on a logarithmic frequency scale, as commonly done to study slow relaxations in glass dynamics [4]. Since the order parameter at the phase transition at $T_c = 0$ is $< X > = \sum_l X_l$, we expect to observe critical slowing down in both $S_{X_l X_k}$ and $\chi''_{X_l X_k}$. The half width of a central peak around $\omega = 0$ in $S_{X_l X_k}(\omega)$ or the position of the corresponding low-frequency peak in $\chi''_{X_l X_k}(\omega)$ could serve as an inverse relaxation time.

Another powerful and mathematically well defined method in studying nonlinear dynamics of complex systems is the Lyapunov spectrum, meaning in our case the set of $2N$ Lyapunov exponents of a one-dimensional N-particle system, ordered with respect to their magnitude $\{\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{2N}\}$. For Hamiltonian systems that are considered here the spectrum is symmetric with respect to zero, i.e., $\lambda_i = -\lambda_{2N-i+1}$ because of the symplectic evolution in the tangent space [9]. In the thermodynamic limit $N \to \infty$ the existence of a smooth distribution of Lyapunov exponents has been numerically verified [10]. Intensive quantities like a Lyapunov density

$$\lambda(x) = \lambda_{i/N}, \quad \frac{i}{N} \to x, \quad N \to \infty \tag{5}$$

or the Kolmogorov-Sinai entropy per particle S_{KS}

$$S_{KS} = \int_0^1 \lambda(x) \, dx \tag{6}$$

can be introduced as useful quantities for the description of the system behavior. In the simplest cases it can be explicitely shown that the value of the positive Lyapunov exponent, which characterizes the correlation decay on short time scales (local instability), is also connected (sometimes linearly) to a relaxation time of the system [11]. In other words, the Lyapunov exponents determine the relaxational behavior of correlators. However in systems with many degrees of freedom the connection between the Lyapunov exponents and the time dependence of correlators on long time scales is not known. In highly chaotic regimes the shape of the function $\lambda(x)$ is always linear and independent of the special form of the Hamiltonian, as was proved by random matrix approximations [12]. As the temperature decreases, decreasing of the KSE occurs due to an increase in the curvature of $\lambda(x)$ and a decrease of λ_1 towards a less chaotic behavior. In the low temperature regime the shape of $\lambda(x)$ around $x = 0.5$ is nestled against the x axis yielding a growing number of very small Lyapunov exponents preparing the smooth transition to the integrable case $S_{KS} = 0$ at $T = 0$. From the special shape of the KSE as function of temperature, we expect to get additional information about the longest time scales of the system with respect to the shortest ones, i.e., about the relaxation behavior. A similar method was used in [13] to detect a phase transition in a two-dimensional Heisenberg model and in Refs. [6, 7] to detect the SST. To evaluate the properties of interest we used molecular dynamics methods. The detailed explanation is given in [14] for the time dependence of correlators and in [15] for the Lyapunov spectra.

III. RESULTS

A. $C = 4$

For $C = 4$ we find the following scenario. With decreasing temperature the inverse correlation length $1/\xi$ decreases. At $T \approx 0.35$, ξ is of the order 200 [16, 14]. At that temperature a drastic change in the temperature dependence of $1/\xi$ (on a linear scale) takes place [14]. On a linear scale (Fig. 1 in [14]) it looks like $1/\xi$ becomes zero below the crossover temperature. However, that is not the case (there is no phase transition at finite temperatures in those systems). Instead the correlation length stays finite at lower temperatures, but it becomes very large. A discontinuity is seen in the inverse static susceptibility at this temperature. The temperature dependence of the position $\omega_{\alpha'}$ of the low frequency relaxational peak in $\chi''_{X_l X_l}(\omega)$ (cf. [14]) is shown in Fig. 1. Clearly a crossover behavior at $T \approx 0.3$ is observed.

In Fig. 2 we show the temperature dependence of the KSE. Again we find a crossover behavior around the same temperature 0.3. The KSE tends to zero by lowering the temperature to the crossover value. Below the crossover the temperature dependence of the KSE is seemingly drastically changed.

The interpretation of the excitation spectrum of the system goes as follows. At temperatures around 0.5 and below, kink-induced relaxations become well separated from (still anharmonic) phonon excitations [17]. The decrease of temperature leads to a decrease of the density of the kinks, thus allowing us to detect their presence in the low-frequency part of the spectrum. Despite the discreteness of the system (lattice) the kinks are not affected by the negligible Peierls-Nabarro potential (the Peierls-Nabarro barrier is $\approx 4 \times 10^{-8}$) and essentially move as in the corresponding continuum system [18]. Because the density of the kink subsystem is low, the collisions between kinks become rare. The increasing relaxation times appear because of lowering the kink density. Only the motion of kinks can provide the system with an equilibration channel. Let us test the applicability of the phonon-kink picture where phonons and kinks are assumed to be noninteracting with each other. Then it follows that the inverse correlation length (or kink density) is proportional to the square root of the inverse temperature multiplied with an exponent of $-E_k/T$, where $E_k = 2/3\sqrt{2C}$ is the minimum kink energy [19]. In Fig. 3 we clearly see how this law is realized. A rough estimation of the kink energy from the slope in Fig. 3 even yields the continuum value within 5% [18]. This result also indicates that the above discussed dynamical crossover is not detected in the simple temperature dependence of the relaxation times and correlation length, but rather in more subtle

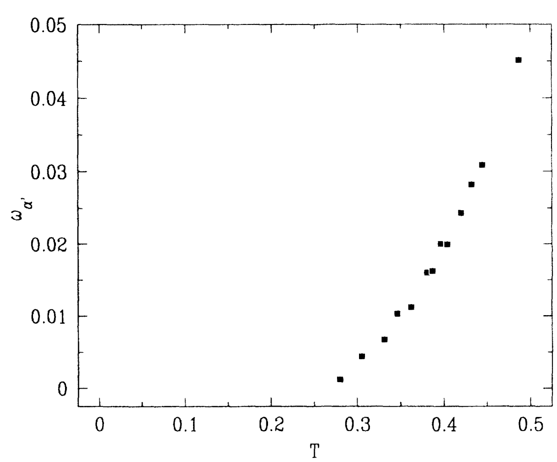

FIG. 1. Position of the low-frequency relaxational peak of $\chi''_{X_l X_l}$ $\omega_{\alpha'}$ (cf. [14]) versus temperature T for $C = 4$, $N = 4000$.

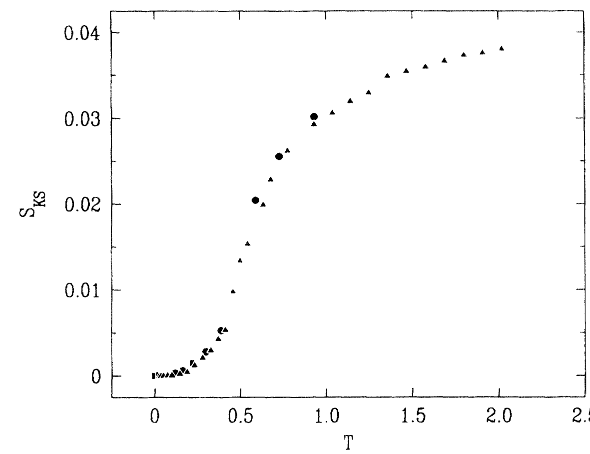

FIG. 2. Kolmogorov-Sinai entropy S_{KS} versus temperature T for $C = 4$. Triangles: $N = 20$; squares: $N = 50$; circles: $N = 100$.

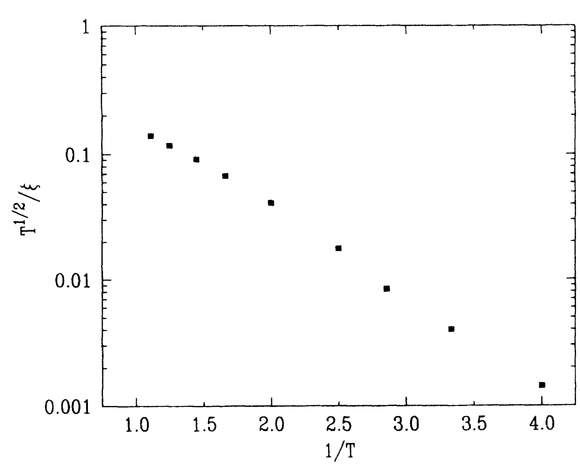

FIG. 3. $T^{0.5}/\xi$ versus $1/T$ for $C = 4$, $N = 4000$.

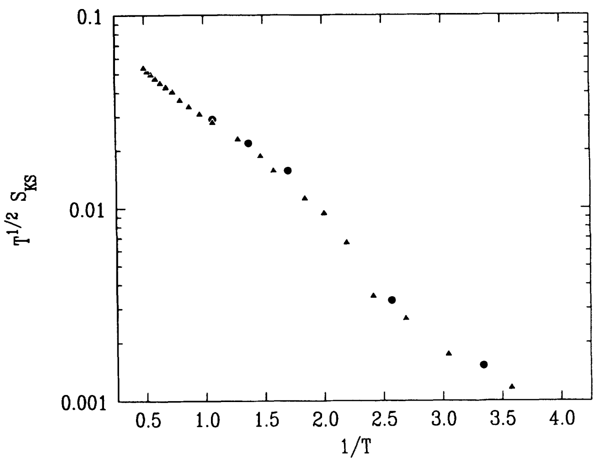

FIG. 4. $T^{0.5}S_{KS}$ versus $1/T$ for $C = 4$. Symbols are the same as in Fig. 2.

dynamical scaling properties [14]. Consequently we expect the same to apply to the KSE. We show in Fig. 4 the realization of the same temperature law as in Fig. 3 for the correlation length. Thus the essential result we find is that the rapid decrease of the KSE below $T = 0.5$ indicates the system to be close to an integrable one. The analysis of the high-frequency excitation spectrum as well as the low-frequency relaxation spectrum leads to the conclusion that the system can be described by a mixture of weakly interacting phonons and kinks with corresponding temperature dependent kink density.

B. $C = 0.1$

For $C = 0.1$ the scenario is changed. The correlation length increases very slowly with decreasing temperature. At $T = 0.1$ it is still of the order of 5 lattice spacings [16, 14]. The relaxation time increases much more rapidly. In [16] it is seen that an analogous crossover temperature as in the $C = 4$ case seems to be reached at temperatures around $T = 0.1$. In Fig. 5 we show $\omega_{\alpha'}$ (cf. [14]) as a function of temperature. Indeed, a strong slowing down is observed around the above cited temperature.

In Fig. 6 the temperature dependence of the KSE is shown. First we find a maximum in the KSE around $T = 0.5$ (for a discussion see [15]). Below that temperature the KSE rapidly decreases with decreasing temperature. That indicates that for $T < 0.5$ one can again try to find an integrable system which is close to the studied one. Second there is a steplike decrease in the KSE at $T \approx 0.03$ (inset in Fig. 6).

The interpretation of the excitation spectrum is not well known in that case. Let us start with the still present kink subsystem. The change of the interaction parameter C from 4 to 0.1 mainly affects the movability of the kinks. That should happen because the Peierls-Nabarro potential that the kinks are affected by during their motion through the lattice has a barrier height of approximately 0.164 [18]. Thus the kinks are trapped by the discreteness of the lattice. The radiation of energy by moving kinks is also strong compared to the $C = 4$ case. Then the lattice site change of a kink becomes a hopping process without strong correlations to previous site changes. Consequently for the same kink densities as in the $C = 4$ case a longer relaxation time of the displacement-displacement correlator can be expected, as found in the numerical simulations [14].

Still the kink density decreases with temperature, so that more and more different degrees of freedom are excited when lowering the temperature. In contrast to the $C = 4$ case the high-frequency part of the displacement-displacement spectrum is far from being described by (weakly interacting) phonons [17, 14]. The spectrum in this frequency range is qualitatively very similar to spectra of uncorrelated particles ($C = 0$) [20]. However this seems to be strange since one can estimate the interaction contribution for $C = 0.1$ and find that in the given temperature (energy) ranges the coupling energy is comparable with the total energy [21]. To understand the nature of this high-frequency part we show in Fig. 7 the time dependence of the local energy-energy correlator for

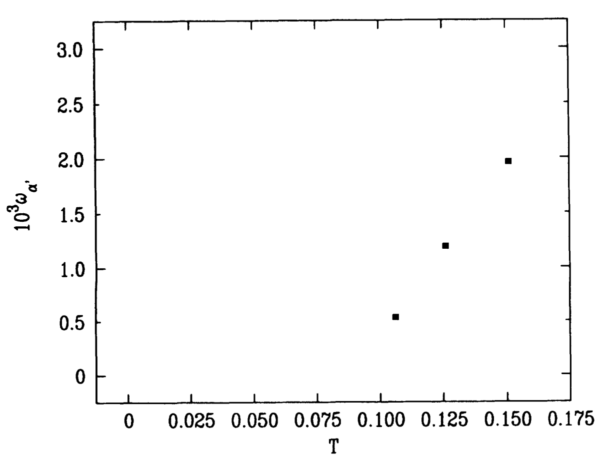

FIG. 5. Same as in Fig. 1 but for $C = 0.1$.

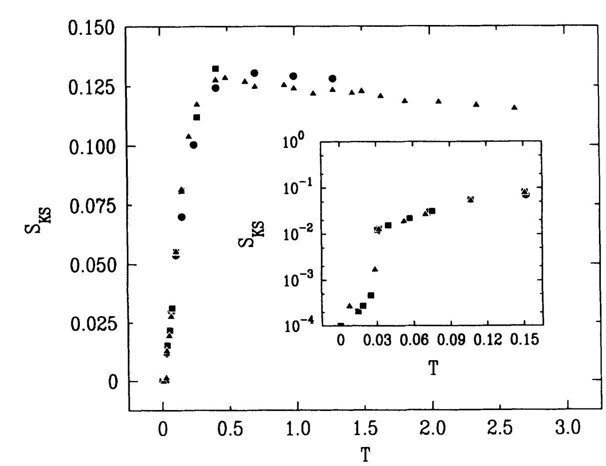

FIG. 6. Same as in Fig. 2 but for $C = 0.1$. Inset: Zoom of the temperature region $0 < T < 0.15$.

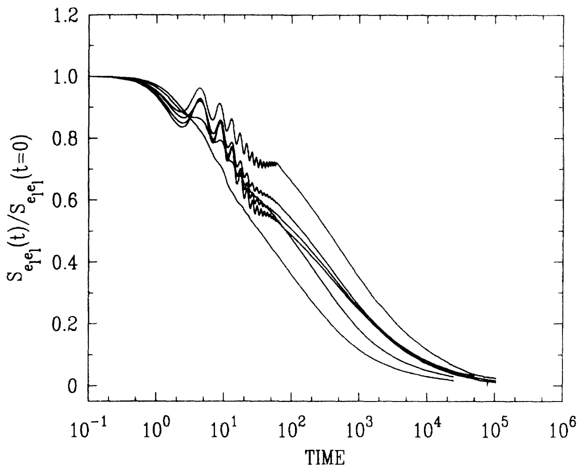

FIG. 7. Local normalized energy-energy correlator $S_{e_l e_l}$ versus time for $C = 0.1$, $N = 1000$ and the temperatures $T = 0.055, 0.067, 0.07, 0.073, 0.11, 0.15$ (lower temperatures correspond to higher values of the correlator at large times).

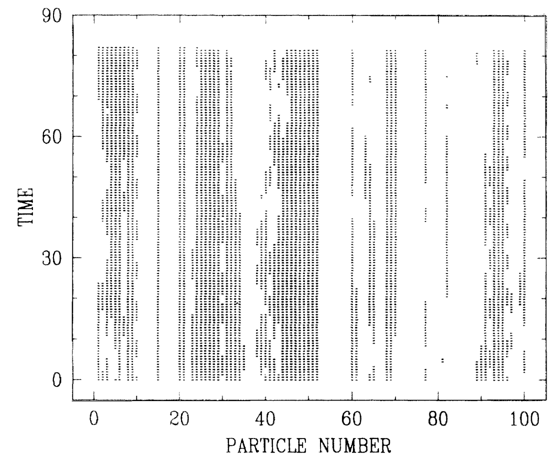

FIG. 8. Hypsometric plot for the displacement patterns for $C = 0.1$, $T = 0.1$, and $N = 1000$. A segment of the chain (100 particles) is actually shown. Ordinate: time; abscissa: particle number. A filled square is drawn if the given particle has negative displacement, otherwise white space is left.

different temperatures, i.e., for

$$A_l = e_l = P_l^2/2 + V(X_l) + 0.25C[(X_l - X_{l-1})^2 + (X_{l+1} - X_l)^2] \ .$$

If the kink excitations are the only localized ones, then we expect a plateau to appear in the correlator. We could estimate the height h_{ee} of the plateau by knowing the kink energy $E_K \approx 0.258$ [18] and the kink density $1/\xi$: $h_{ee} = E_K^2/(2\xi)$. For all temperatures in Fig. 7 we find that we underestimate the height of the plateau by 30–50 %. Thus we have to conclude that other degrees of freedom in the system are excited, which provide energy localization. The explanation of the puzzle is very likely the existence of nonlinear localized excitations (NLE's) [22,21]. These NLE's can be excited without the presence of topologically induced kinks as well as in combination with kinks. The NLE's are (nearly) regular solutions of the nonlinear translationally invariant lattice. A single NLE is described by a finite set of fundamental frequencies and can be viewed as the excitation of a finite set of nonlinear localized degrees of freedom. Thus a given lattice which shows up with NLE's at finite temperatures can be viewed as evolving (close to) on high-dimensional tori in phase space for finite times. The typical NLE for the case under study consists of three excited particles, one central (large amplitude), and two neighbors (small amplitudes). Indeed the NLE's can be observed in hypsometric plots in [14]. In Figs. 8 and 9 we show two hypsometric plots which demonstrate the presence of NLE's at the temperature $T = 0.1$. Finally in Fig. 10 we show $\chi''_{e_l e_l}$ versus frequency. The huge halfwidth of the low-frequency relaxational peak (nearly three decades) indicates that several relaxational processes are present, e.g., the kink hopping and the NLE relaxation. There are two intriguing facts which support the above given interpretation of the spectrum. First it is known that the NLE's (excluding the NLE's excited on kinks) have an existence energy threshold [22]. For $C = 0.1$ this threshold has a value of about $E = 0.1$ [22]. Since three particles are involved in the NLE, it yields an energy of 0.03 per particle. This value comes rather close to the above described step in the KSE at $T = 0.03$. The reason why the KSE *increases* steplike if one heats the system above the step temperature might be that below $T = 0.03$ essentially no NLE's are excited, so the system excites small amplitude phonons which can have longer lifetimes compared to the NLE's. Above the step temperature more NLE's are excited. The second fact is that the NLE's completely disappear at NLE energies of around 1.5 [21]. This corresponds to an energy per particle of 0.5. It is rather close to the found maximum in the KSE at $T = 0.4$.

IV. DISCUSSION

When the KSE of a system becomes zero at a certain value of the system control parameter, the system itself

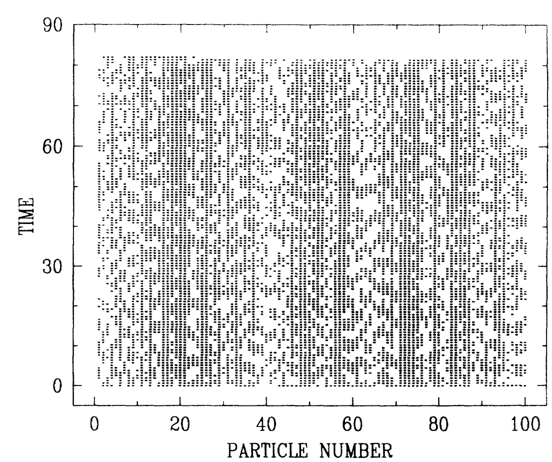

FIG. 9. Same as in Fig. 8 but a filled square is drawn if the displacement of the given particle is closer to any of the ground state positions ± 1 than 0.3.

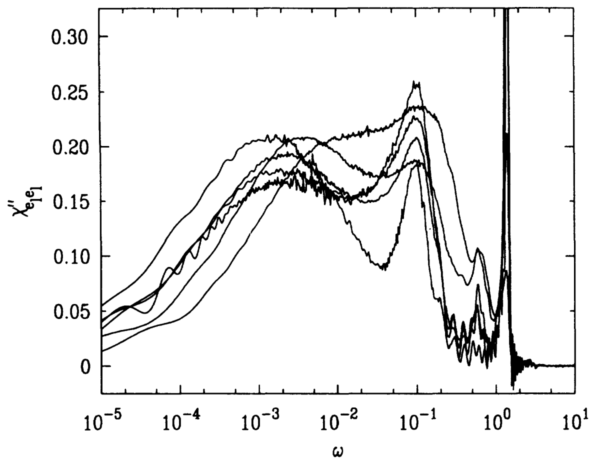

FIG. 10. $\chi''_{e_l e_l}$ for $C = 0.1$, $N = 1000$ versus frequency ω as calculated from the correlators in Fig. 7. Lower temperatures correspond to lower values of the position of the lowest-frequency relaxational peak.

becomes integrable. If the KSE tends to zero (but does not exactly become zero) approaching a certain range of the control parameter space, the system becomes close to an integrable system. Our results show that for the one-dimensional Φ^4 system at the same time as the temperature dependence of the KSE shows up with a crossover, the temperature dependence of certain relaxation times of the system does the same. What that result implies is that if the relaxation of a system drastically slows down, the system itself becomes drastically close to an integrable system. That means that the system evolves over longer and longer times close to some tori in the phase space, and mixing occurs on larger time scales. The mixing time scale which should be essentially identical with the relaxation time becomes separated from the time scale provided by the motion on the tori of the corresponding integrable system (i.e., the inverse frequencies in the action-angle representation of the integrable system).

Now we can formulate an essential part of our results. If the relaxation time of a system becomes drastically large (by smooth changes of control parameters) that would imply that certain Lyapunov coefficients may tend to zero. But surprisingly we find that the largest Lyapunov coefficient tends to zero, and thus the whole KSE. Consequently the whole system becomes close to an integrable system.

In analyzing the data for $C = 4$ we found that in the temperature region of low KSE and large relaxation times the system becomes close to a weakly interacting kink-phonon system. Thus our analysis provides us with an understanding of the typical "quasiparticles" (phonons, kinks) and the reasons for slow relaxation (low kink density, weak phonon-phonon interaction). The $C = 0.1$ case turns out to be similar in the correlation between KSE and relaxation, but totally different in the interpretation of the excitation spectrum. Here our analysis supports the picture of nonlinear localized excitations as quasiparticles together with kinks. The slow relaxation is now given by the slow diffusion of kinks (high Peierls-Nabarro barrier) and the slow relaxation and interaction of NLE's.

Butera and Caravati [13] have found numerically that a system of the Heisenberg O(2) universality class shows up with a crossover of the maximum Lyapunov coefficient versus temperature behavior at the phase transition (where both correlation length and relaxation times diverge). This result could be viewed in analogy to our $C = 4$ case. Undoubtedly the system becomes nonergodic if one passes the critical temperature from above. The strange part in both results is the following: the fact that the largest Lyapunov coefficient (and thus the KSE) tend to zero at the critical point implies the system to be close to an integrable one.

Let us also mention the results of Pettini and Landolfi [6] and Pettini [7]. These authors have investigated a modified Φ^4 model [where $V(X) = \frac{1}{2}X^2 + \frac{1}{4}X^4$] and Fermi-Pasta-Ulam models in one dimension. All these models seem not to have a phase transition, thus the found slowing down cannot be attributed to large spatial correlations. The observed crossover both in the relaxation times and in the largest Lyapunov exponent versus temperature dependence were thus attributed to the presence of a strong stochasticity threshold. This threshold separates motion mainly along resonances from motion mainly across resonances of an assumed underlying and perturbed integrable system.

Another interesting case is the study of liquid-glass transitions. These transitions are defined by a slowing down of structural relaxation in the undercooled liquid. Recently Madan and Keyes [23] have studied the dynamics of Lennard-Jones liquids. Using molecular dynamics they calculated the fraction of unstable modes out of an averaged density of states. Around the freezing (glass) transition a crossover in the temperature dependence of the fraction of unstable modes is found. Although there is no clear mathematical connection between their density of states and the Lyapunov spectrum, it seems to be likely that an investigation of the largest Lyapunov exponent would yield analogous results.

Summarizing we have shown two examples of slowing down in complex systems. The simultaneous decrease of the KSE allows us to make statements about the nature of excitations in the systems under consideration. Below the crossover (dynamical phase transition, strong stochasticity threshold) the systems are likely to behave as a set of weakly interacting excitations. Thus one can construct microscopic theories to describe the crossover phenomena.

Note added. We have recently learned about systematic discrepancies between the behavior of the correlation length in the case $C = 4$ and results from considerations of noninteracting kinks and phonons [24]. However these discrepancies do not indicate in any form a dynamical crossover mediated by the kink-phonon interaction. Consequently the results on the phonon-mediated effective kink-kink interaction of Ruderman-Kittel-Kasuya-Yosida–type as found in [25] should not alter our observations. Finally let us mention the observation of NLE-type excitations at finite temperatures in a new Klein-Gordon chain with double-quadratic onsite potentials [26].

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