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Dynamical properties of one-dimensional Lennard–Jones lattice

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Abstract

We report the dynamical instability of one-dimensional chain with nearest-neighbor Lennard–Jones interaction. It is found that a certain plateau region exists in the energy dependence of the maximal Lyapunov exponent between weakly and strongly chaotic regions. That is, the exponent is insensitive in the region to the increase of the total energy of the system. It is numerically shown that the region is enhanced with the decrease in the particle density. The spatio-temporal patterns of particle position in the region shows a kind of collective motion, especially for low particle density cases. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction and models

Dynamical properties of one-dimensional (1-D) system with large number of degrees of freedom, such as FPU model and ϕ^4 model, have been extensively investigated since the original studies [1,8,9]. However, 1-D Lennard–Jones (LJ) chain has not been studied except for some early works in the 1970s [2], although it retains basic interest in the nonlinear dynamics.

Our purpose is to investigate the specific energy (i.e., energy density) dependence and the particle density dependence of the maximal Lyapunov exponent (MLE) in LJ system. We deal with a one-dimensional N particle system confined within an interval L described by the following Hamiltonian:

$$H = \sum_{n=1}^{N} \left[\frac{p_n^2}{2} + U(|u_{n+1} - u_n|) \right], \tag{1}$$

where u_n and p_n are the coordinate of the nth atom and the conjugate momentum, respectively, and U is the LJ pair potential between the nearest-neighbor atoms, which is given by

$$U(r) = 4\left[\left(\frac{1}{r}\right)^{12} - \left(\frac{1}{r}\right)^{6} \right] + f(L,N). \tag{2}$$

The $f(L,N)$ is taken to be a constant which makes the total potential energy zero. The periodic boundary condition is used. The potential minimum is given at $r_0 = 2^{1/6}$. We set the particle density d unity when all particles are arranged with equal interval r_0, i.e., $d = Nr_0/L$. When the system length L is changed while keeping the number of particles, the configuration of the equilibrium state becomes

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quite a different one from the configuration with equal interval.

2. Numerical result and discussion

We have used 6th order symplectic integrator with a small time step to integrate numerically the equations of motion for various system parameters such as the particle density d and the specific energy E [3]. The energy dependence of MLE, which is an indicator for stochasticity, can be calculated by the time evolution of an infinitesimal perturbation vector $\xi(t) = (\delta p_1(t), \ldots, \delta p_N(t), \delta q_1(t), \ldots, \delta q_N(t))$ in $2N$ dimensional tangent vector space. The MLE λ_1 is roughly given by $\lim_{t\to\infty}|\phi(t)| \propto \exp(\lambda_1 t)$, where the $|\phi(t)|$ is proportional to a norm $\|\boldsymbol{\delta\xi}(t)\|$.

Fig. 1 shows the energy dependence of the MLE λ_1 at various particle densities d. A certain plateau region (P-region) exists between the quasiperiodic (solid-like) region corresponding to $E \ll E_1$ and

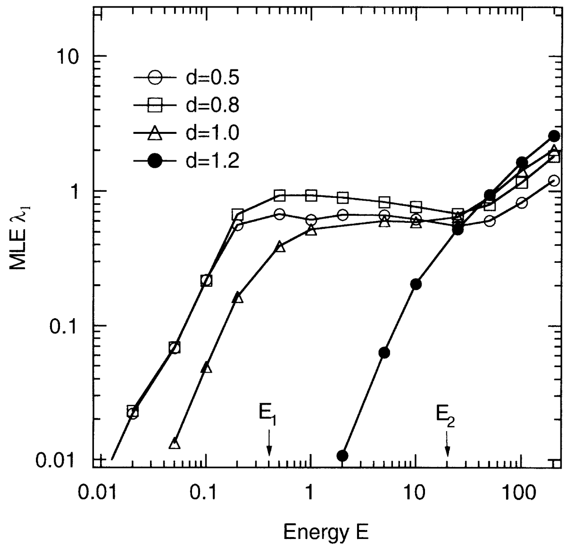

Fig. 1. Log–log plot of MLE $\lambda_1(E)$ as a function of specific energy at various densities in Lennard–Jones system. The arrows roughly show $E_1 = 0.4$ and $E_2 = 20$ to distinguish three regions.

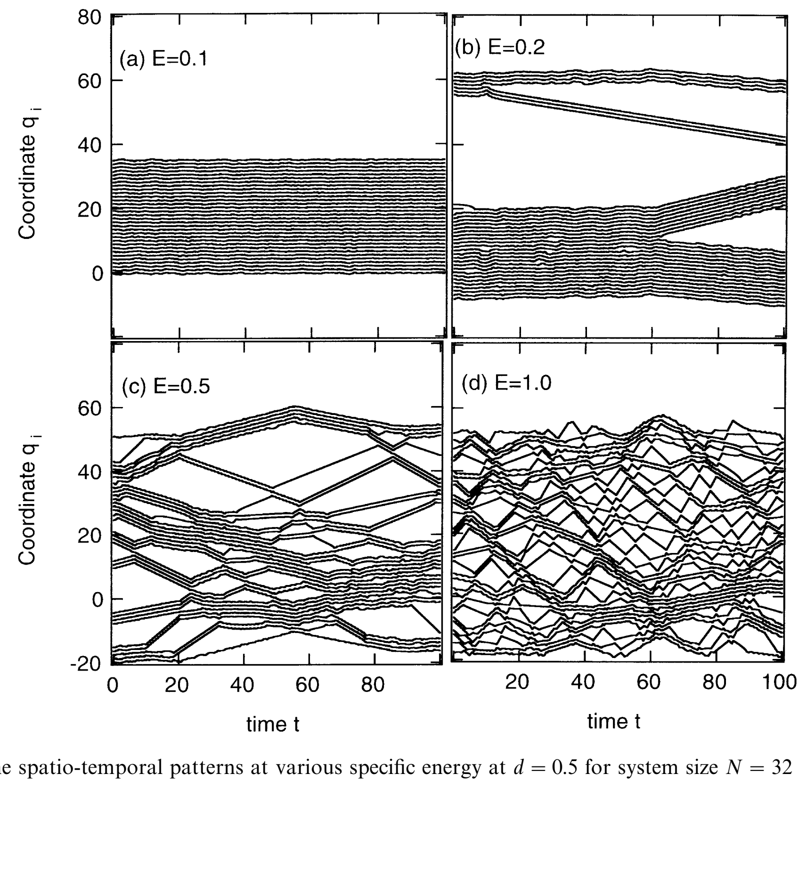

Fig. 2. Some spatio-temporal patterns at various specific energy at $d = 0.5$ for system size $N = 32$ in LJ system.

strongly chaotic (gas-like) region corresponding to $E > E_2$. In that region the energy dependence is insensitive to the increase of the specific energy. The presence of the P-region ($E_1 \ll E < E_2$) is a remarkable feature in LJ system, different from FPU or soft-core system in which the potential form has convexity for the entire specific energy region [4]. On the other hand, when we pay attention to the particle density dependence of λ_1, it follows that a clear P-region is well-observed in low density cases $d < 1$, and P-region disappears in high density cases $d > 1$.

There are two types of mechanism which cause exponential instability. The first type causes local instability and the other parametric instability (global instability). If the potential form is convex such as FPU or soft-core type, only parametric instability exists in the system. On the other hand, since both types of instabilitiy exist in the LJ system, the local instability is regarded as a cause to generate P-region [4]. Moreover, there are also the two types of mechanism, parametric and local instabilities, in the Morse system [5]. A P-region can also be well observed in the energy dependence of the MLE λ_1 in the Morse system. Accordingly, these facts support that the presence of local instability is an effective cause of the existence of the P-region. More details of numerical results will be shown in Refs. [6,7].

The existance of the P-region means that the increase in the specific energy does not increase stochastic orbits immediately in the region. It is supposed that the energy is used to generate co-operative motions in the region. Fig. 2 shows some spatio-temporal patterns of the particle position at several energies for $d = 0.5$. In fact, a (clustered state like) co-operative particle motion can be well observed [6,7].

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