Lyapunov Analysis of One-Dimensional Lennard-Jones System

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We report characteristic energy dependence of dynamical instability in the one-dimensional Lennard-Jones system. We compare the results with those of Fermi-Pasta-Ulam system.

We have already reported energy-dependence of maximum Lyapunov exponent (MLE) in one-dimensional Lennard-Jones (LJ) system.\(^1\)-\(^3\) As a result, the energy-dependence is classified into four characteristic regions as the energy of the system increases: (1) quasiperiodic, (2) weakly chaotic, (3) plateau and (4) strongly chaotic regions.\(^1\)-\(^3\) The existence of the plateau region, in which the energy-dependence is insensitive, is a remarkable feature of LJ system, different from Fermi-Pasta-Ulam (FPU) and soft-core system. (See Fig. 1.)

In this report, we give the details of the characteristics of dynamical property in the plateau region, by calculating distribution of local MLE with comparing with FPU system.

\[ E_K \equiv \frac{K}{N}, \]

where \( K \) and \( N \) are the total kinetic energy and the particle number, respectively. (a) in LJ system and (b) in FPU system. Numerical convergency has been confirmed for various initial conditions. Some specific kinetic energy \( E_K \) used in Fig. 2 are shown by arrows.

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We define local Lyapunov exponents \{[\lambda_i \tau], i = 1, \cdots, 2N\} for finite time interval \(\tau\) by means of time-evolution of eigenvalues of real symmetric symplectic matrix. Figure 2(a) is the distribution of local MLE \([\lambda_1]_\tau\). A drastic change appears in the distribution between weakly chaotic region and plateau region. In the weakly chaotic region \((E_k = 0.046)\) the distribution form is almost Gaussian, on the other hand, in the plateau region \((E_k = 0.91)\) a sharp peak appears around \([\lambda_1]_\tau \approx 6\) and the other part distributes flatly. We call the peak first peak in order to distinguish from second peak which begins to appear in strongly chaotic region. The distribution in FPU system is given in Fig. 2(b). It is evident that the distribution form is almost Gaussian for any energy.

We have investigated an exponent \(\lambda_A^{\max}\) which is defined based on local instability of the system, \(\lambda_A^{\max} = \sqrt{\alpha_{\min}(t)}\) where \(\alpha_{\min}\) is a minimum negative eigenvalue of the Hessian matrix of the total potential function. In FPU system, there is no local instability \(\lambda_A^{\max}\) because the total potential function is convex function. As a result, it has been suggested that the first peak in the distribution of local MLE is strongly related to the local instability. The details are given in Refs. 4) and 5).

References