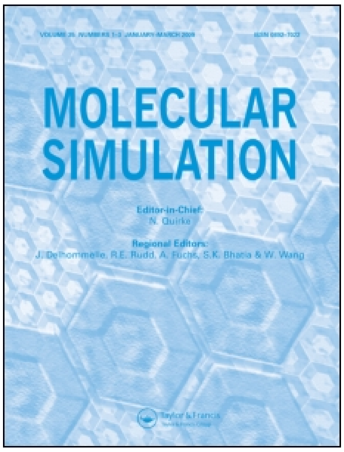

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

Irreversibility and Interatomic Potentials in One-dimensional Lattice Models

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To cite this Article Machida, Masahiko and Kaburaki, Hideo(1994) 'Irreversibility and Interatomic Potentials in One-dimensional Lattice Models', Molecular Simulation, 12: 3, 435 — 439
To link to this Article: DOI: 10.1080/08927029408023051
URL: http://dx.doi.org/10.1080/08927029408023051

Molecular Simulation, 1994, Vol. 12(3-6), pp. 435–439
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Note

IRREVERSIBILITY AND INTERATOMIC POTENTIALS IN ONE-DIMENSIONAL LATTICE MODELS

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(Received March 1993, accepted July 1993)

KEY WORDS: Chaotic motion, diatomic toda lattice, FPU model, separation distance, thermal conduction

Since the computational work on the relaxation process toward the equilibrium state by Fermi, Pasta, and Ulam (FPU) [1] , the stochastic behaviors in one dimensional lattice models have been studied by many physicists numerically and theoretically. The objective of those studies is to understand the origin of thermodynamical properties from the microscopic particle motions which are determined by the deterministic equations of motion. In the FPU work, since the given energy was too small and anharmonicity was too weak, thermodynamic irreversibility phenomena, which lead to the equipartition of energy among modes, were not observed. Many studies after this work confirmed the existence of the threshold for the chaotic motions [2] [3]. However, the relation of the chaotic motion in the system with many degrees of freedom to the thermodynamical properties is not well understood [4]. The steady lattice thermal conduction in one dimensional lattice poses an interesting problem in this; respect. A clear linear internal temperature gradient was not observed in the FPU model [5], while it was observed in the the ding-a-ling model by Casati *et al.* [6] and the diatomic Toda lattice (DTL) by Mokross and Büttner [7]. Recently, the system size dependence of the coefficient of thermal conductivity has been studied [8][9] and the Fourier's law of heat conduction is begining to be confirmed in the DTL.

In this paper, for the purpose of understanding the mechanism of this lattice thermal conduction, computer simulations of one dimensional Hamiltonian systems for three different lattice models (DTL, FPU, and diatomic FPU(DFPU)) are made to clarify the difference in chaotic motions. In the numerical simulations, the separation distance ($D(t)$) in the phase space for the initially close orbits is

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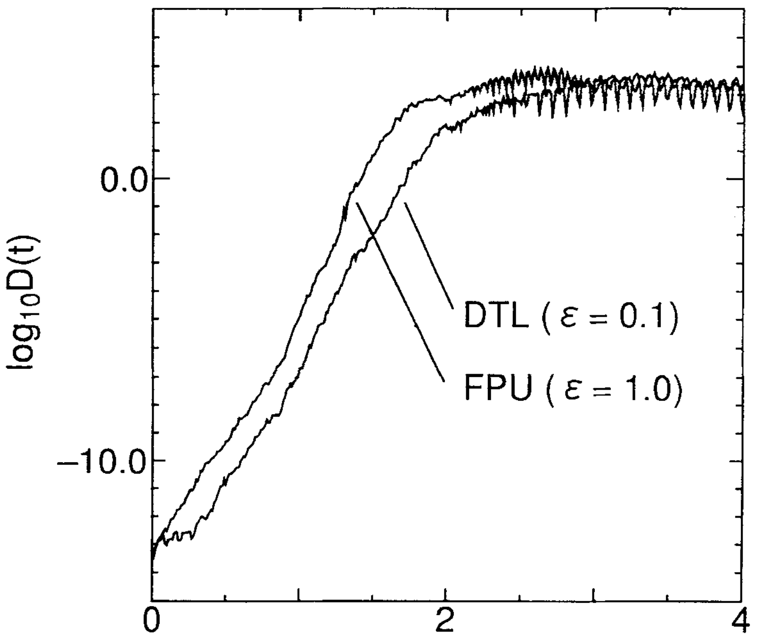

Figure 1 The comparison of the separation distances $D(t)$ for the DTL and FPU models at the energy density of $\varepsilon = 0.1$ for DTL and $\varepsilon = 1.0$ for FPU.

measured to detect the chaotic motion and also to estimate the strength of stochasticity [10]. The $D(t)$ is defined as follows:

$$D(t) = \sqrt{\sum_{i=1}^{N} (x_i'(t) - x_i(t))^2 + \sum_{i=1}^{N} (p_i'(t) - p_i(t))^2}, \tag{1}$$

where N is the total number of particles and x_i and p_i are the displacement and the momentum of the i-th particle, respectively. The primes for x_i and p_i indicate that these values are slightly different from the umprimed ones in the initial state. Although $D(t)$ is generally dependent upon the initial conditions, it becomes insensitive for the strong chaotic motion [11]. The behavior of $D(t)$ is considered to be a good strong chaotic detector for the system with many degrees of freedom. The value of $D(t)$ increases linearly if the motion is stable, but it grows exponentially if the motion becomes unstable and chaotic. It is also known that the two systems with the same rate of exponential growth show similar statistical behaviors.

For the numerical integration of the equations of motion, a new integration method, which is derived from the general theory for the decomposition of exponential opreator [12], is used. The advantage of this method is that the energy conservation for an arbitrary precision is guaranteed theoretically and that the algorithm is easier to program than other methods such as the Runge-Kutta method.

The scaled model Hamiltonians for the DTL and FPU models are as follows:

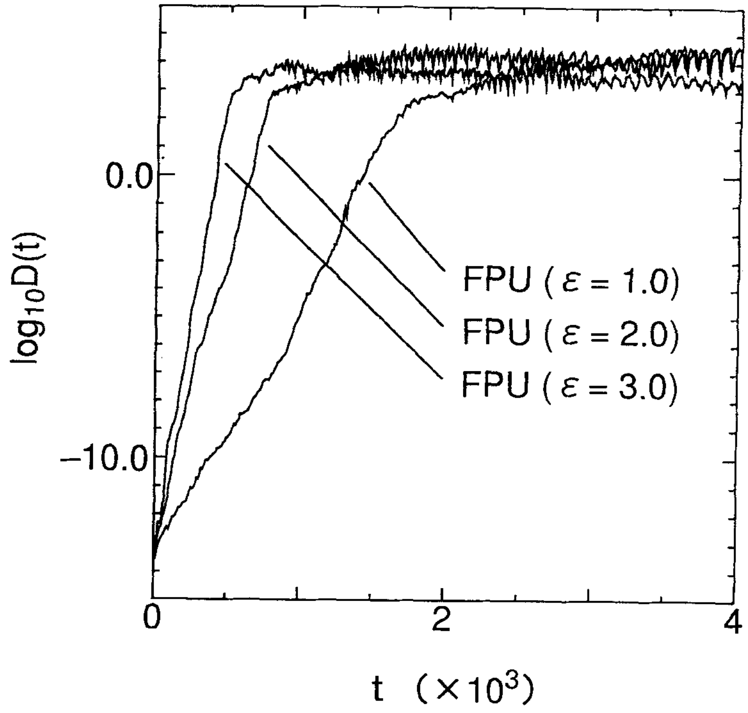

Figure 2 The effect of the energy density for the FPU model.

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \frac{1}{\alpha^2} \sum_{i=0}^{N} \{\exp(-\alpha r_i) - \alpha r_i\}, \quad r_i = x_{i+1} - x_i \tag{2}$$

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i=0}^{N} \left\{\frac{1}{2} r_i^2 + \frac{1}{24} r_i^4\right\}, \quad r_i = x_{i+1} - x_i \tag{3}$$

where the values of x_0 and x_{N+1} are fixed zero and the total energy is conserved. In the simulations, the nonlinear parameter α is set equal to unity. The FPU Hamiltonian is derived from expanding the Toda potential for the small r_i and retainning only the fourth order term. The lattice is called as diatomic when the masses at the odd number lattice sites are replaced by half the mass of the host atom. In the region of the strong chaotic motion, the exponential growth of $D(t)$ is characterized by h which is a measure of the strength of stochasticity.

$$D(t) = D(0)\exp(ht) \tag{4}$$

In strong stochastic motions, the dependence of the initial conditions can be neglected. Computer simulations are made for the system consisting of 100 atoms. Figure 1 shows the temporal behavior of $D(t)$ for the DTL and FPU models. Here, the energy density ε, which is the energy per one atom, is assumed to be 0.1 for the DTL model and 1.0 for the FPU model. The separation distance in both models

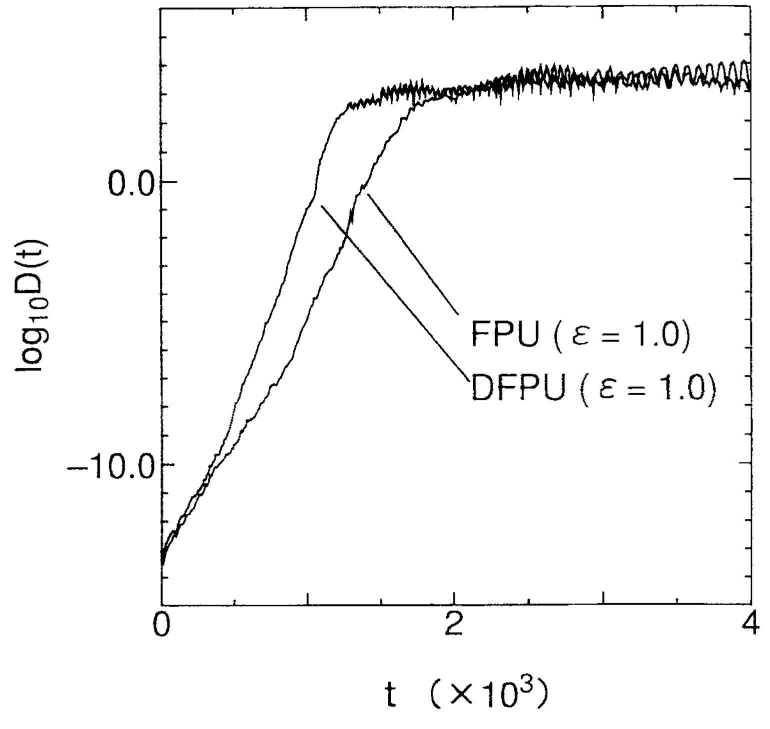

Figure 3 The comparison of the FPU and the DFPU model for the same energy density $\varepsilon = 1.0$.

shows exponential growth from the outset and comes to a constant value. It is also seen that both cases show almost the same h. This means that the DTL model shows stronger chaotic motions than the FPU model for the same energy density. Figure 2 shows the behavior of $D(t)$ for the FPU model with three different values of ε. As the energy density increases, it is seen that the value of h increases and thus the stochasticity of the system increases. Figure 3 shows the difference of the FPU and DFPU models for the same energy density. The nonuniformity of the mass distribution leads to the enhancement of stochasticity. With the above results, it is predicted that the nonlinearity of the potential is the main cause of the strength of stochasticity. The effect of the nonuniformity of mass distribution is small compared with that of the nonlinearity of the potential.

From the results of $D(t)$, the strong chaotic motions, in which $D(t)$ shows exponential growth, are found for three different (DTL, FPU, and DFPU) models in the high energy density region. The nonlinearity of the potential and the nonuniformity of the mass distribution affect the growth rate h. It is found that the nonlinearity of the potential is important for the system to show strong stochasticity.

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