Stochastic behavior in systems with a Lennard–Jones potential and with only a few particles

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A stochastic behavior has been observed in a system of three particles bound by a Lennard–Jones potential. The conditions under which the invariant tori are destroyed, and the phase trajectories become divergent, are found.

In a landmark paper,[1] Hénon and Heiles first demonstrated the existence of a stochastic behavior in a system of three stars whose behavior is described by a system of nonlinear equations.

There is obvious interest in learning about the behavior of dynamic systems of

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particles which interact with each other via potentials which are approximations of real intermolecular potentials. One such potential is the Lennard–Jones potential

$$U(r) = 4\epsilon[(\sigma/r)^2 - (\sigma/r)^6]. \tag{1}$$

Casartelli *et al.*[2] have shown that a stochastic behavior can occur in one-dimensional Lennard–Jones systems with more than ten particles. We have suggested that a dynamic chaos should prevail even in a system of three particles with potential (1). We have studied the onset of dynamic chaos in such a system on the basis of the divergence of phase trajectories and also by means of Poincaré mappings.

We set $\epsilon = 1$ and $\sigma = 2^{-1/6}$ in potential (1). We set the masses of the particles equal to one ($m = 1$). The Hamiltonian of this system of three particles can then be

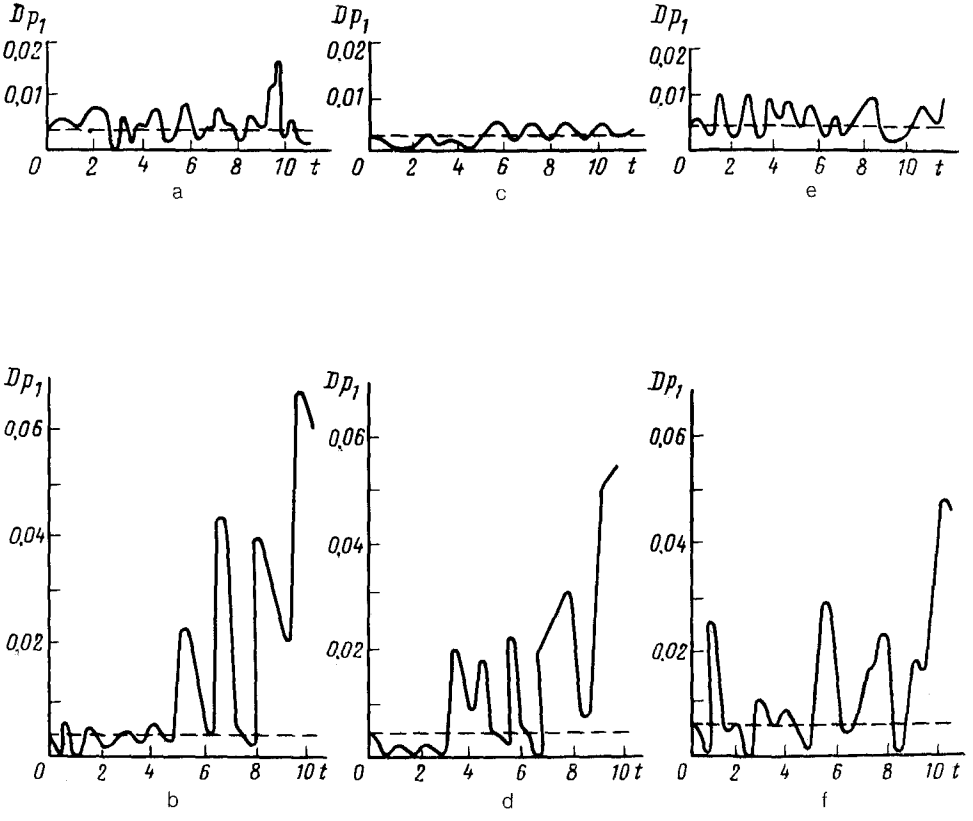

FIG. 1. Dynamics of $D_{p_1}(t)$ in a system of three particles. The values of the initial coordinates q_i are the same in all cases. For version 1 of the initial conditions, the ratios of the initial momenta of the particles for the trajectory from which $D(0)$ is reckoned were $p_1{:}p_2{:}p_3 = 1{:}(-1){:}0$. *a*—$E = -1.64$; *b*—$E = -1.51$. For version 2 of the initial conditions, the ratios of the initial momenta of the particle were $1/\sqrt{3}{:}1/\sqrt{3}{:}(-2/\sqrt{3})$. *c*—$E = -1.84$; *d*—$E = -1.64$. For version 3 of the initial conditions, the ratios of the initial momenta of the particles were $1/\sqrt{3}{:}(-2/\sqrt{3}){:}1/\sqrt{3}$. *e*—$E = -1.36$; *f*—$E = -1.19$. The dashed line is the level of the initial deviation $D(0)$.

written

$$\mathcal{H} = \frac{1}{2}(p_1^2 + p_2^2 + p_3^2)^{-12} + (q_2 - q_1)^{-12} + (q_3 - q_2)^{-12}$$
$$- 2(q_2 - q_1)^{-6} - 2(q_3 - q_2)^{-6}. \qquad (2)$$

We have studied the behavior of system (2) at various values of its total energy E. The equations were integrated numerically by the fourth-order Runge–Kutta method. The time step was chosen to be $\Delta t = 10^{-3}$. The total momentum of the system was zero. The observation time t was $\sim 10^4 \Delta t$.

Figure 1 shows the dynamics of the distances $D(t)$ between the coordinates of the system in phase space for various versions of the initial conditions. Everywhere, the dashed line is the level of the initial deviation $\delta = D(0)$ along the coordinate p_1. We see that at low values of the energy E, for each version considered, the quantity $D(t)$ remains on the order of $D(0)$ over observation times $t \sim 10$. With increasing E, the trajectories diverge. At $E = -1.19$, the divergence of $D(t)$ is observed for all versions of the initial conditions. The divergence of $D(t)$ thus depends on the initial positions of the points in phase space. In the initial stage of the divergence of the trajectories, the ratio $D(t)/D(0)$ is essentially independent of $D(0)$. At large values of t, the trajectories move away from each other rapidly, within the allowed region of phase space.

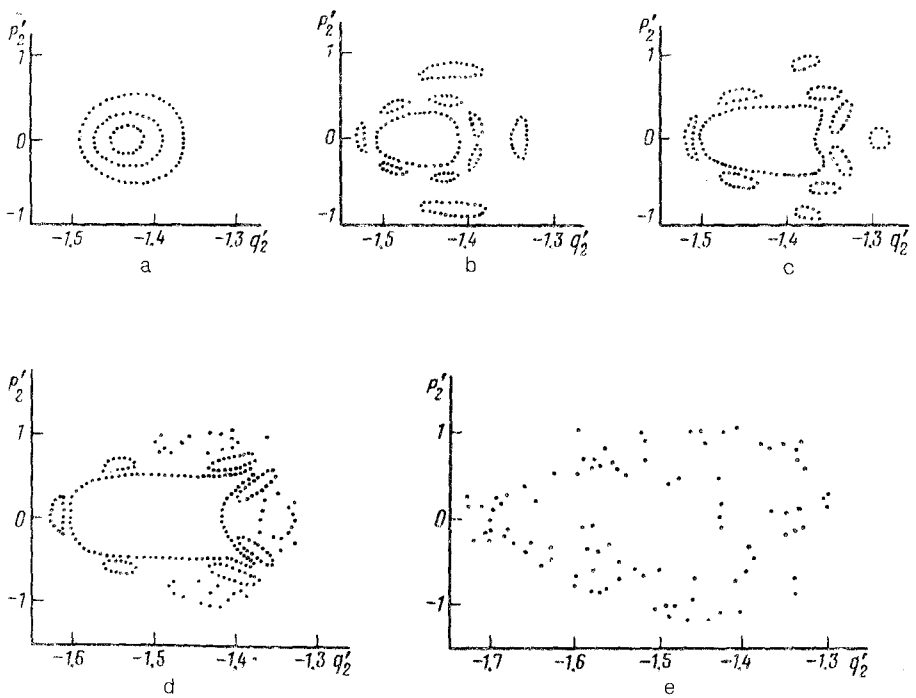

FIG. 2. Poincaré mappings for various values of the energy for the three versions of the initial conditions. *a*—$E = -1.84$; *b*—$E = -1.64$; *c*—$E = -1.51$; *d*—$E = -1.36$; *e*—$E = -1.19$.

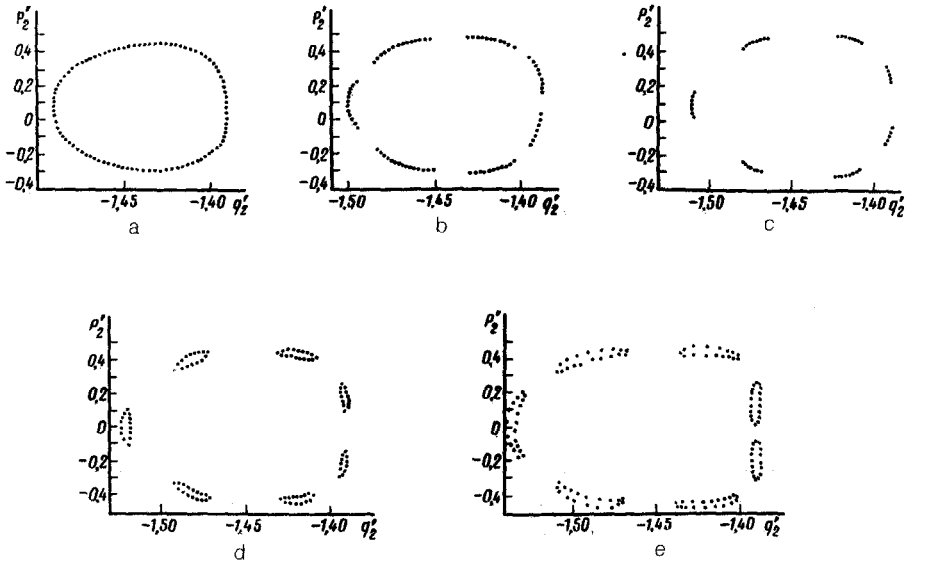

FIG. 3. Poincaré mappings for version 1 of the initial conditions. *a*—$E = -1.77$; *b*—$E = -1.73$; *c*—$E = -1.70$; *d*—$E = -1.64$; *e*—$E = -1.62$.

We now perform a linear orthogonal transformation of the coordinates and momenta in the system with Hamiltonian (2) (Ref. 3). As a result, the Hamiltonian becomes

$$\mathcal{H} = \frac{1}{2}(p_1'^2+p_2'^2)+64[(\sqrt{3}q_1'+q_2')^{-12}+(\sqrt{3}q_1'-q_2')^{-12}]$$

$$-16[(\sqrt{3}q_1'+q_2')^{-6}+(\sqrt{3}q_1'-q_2')^{-6}], \qquad (3)$$

where p_1', p_2', q_1', and q_2' can be thought of as the momenta and coordinates of new particles.

In solving the system of Hamilton's equations, we considered sets of points in the phase space of the second particle which were obtained when the conditions $q_1' = 0$, $p_1' > 0$ were satisfied for the first particle. These conditions correspond to a Poincaré mapping onto the (q_2', p_2') plane.

The results of these calculations are shown in Fig. 2. We studied a total of three versions of the initial conditions for each value of E. We see that at $E = -1.84$ the sets of points of the Poincaré mappings are closed curves. At $E = -1.64$, $E = -1.51$, and $E = -1.36$, some of the curves become deformed, while others break up to some extent. At $E = -1.19$, all the curves disintegrate; i.e., the tori are destroyed. The meaning here is that the destruction of the invariant tori in a system with Hamiltonian (3) occurs at those values of E at which the trajectories diverge (Fig. 1). Direct calculations lead to values greater than zero for the Lyapunov exponents under these conditions.

We also studied the behavior of a system with Hamiltonian (3) at energies near the threshold for the destruction of the tori. Corresponding Poincaré mappings are shown in Fig. 3. At $E = -1.84$, the mapping points in the phase space of the second particle uniformly fill the cross section of a torus. As E increases, the points begin to bunch in seven distinct regions (Fig. 3, b and c). These regions subsequently evolve into seven islands (Fig. 3, d and e). As a result, the initial curve is destroyed; at $E = -1.19$ (Fig. 3e), all the islands are also destroyed. In our opinion, Poincaré mappings give a clearer picture of the transition to a stochastic behavior. In numerical simulations carried out by us with systems of five and seven particles, we found results analogous to those on the three-particle problem. It can thus be asserted that even the three-particle system embodies the basic features of the stochastic behavior of many-particle systems with a Lennard–Jones potential.

[1] M. Hénon and C. Heiles, Astron. J. **69**, 73 (1964).
[2] M. Casartelli, E. Diana, L. Galgani, and A. Scott, Phys. Rev. A **13**, 1921 (1976).
[3] M. Toda, *Theory of Nonlinear Lattices*, Springer, Berlin, 1981.

Translated by D. Parsons