Relaxation to equilibrium in few-particle adiabatic piston systems

Haihong Li,[1] Dahai He,[1] Zhoujian Cao,[1] Ying Zhang,[1] Toyonori Munakata,[2] and Gang Hu[3,1,4,*]
[1]*Department of Physics, Beijing Normal University, Beijing 100875, China*
[2]*Department of Applied Mathematics and Physics, Graduate School of Informatics, Kyoto University, Kyoto 606-8501, Japan*
[3]*China Center for Advanced Science and Technology (CCAST) (World Laboratory), P. O. Box 8730, Beijing 100080, China*
[4]*Beijing-Hong Kong-Singapore Joint Center of Nonlinear and Complex Systems, Beijing Normal University Branch, Beijing 100875, China*

(Received 24 March 2004; revised manuscript received 23 November 2004; published 10 June 2005)

A Hamiltonian system with few particles and a heavy adiabatic piston is studied. With ensemble averages based on proper classification of slow and fast variables, a nonequilibrium state is defined and the relaxation from nonequilibrium to equilibrium is investigated. Coherent oscillation, dissipative oscillation damping, and anti-intuition energy transfer of the adiabatic piston are observed by numerical simulations. Noise-driven thermodynamic equations of slow variables are derived, based on the assumption of local equilibrium and the fluctuation-dissipation theorem, to understand and quantitatively reproduce all the above few-body nonequilibrium relaxation features.

DOI: 10.1103/PhysRevE.71.061103 PACS number(s): 05.20.Jj, 03.75.Hh, 05.45.Ac

I. INTRODUCTION

The problem of statistical behavior of few-body systems has attracted great attention in recent decades. The crucial significance of this topic is that the investigation can build up a bridge from mechanics to statistical physics [1–9] It turns to be clear that a nonlinear mechanical system with few particles may show ergodicity in energy surface, and various thermodynamic quantities can be defined accordingly, and the thermodynamic second law can be applied to such a system, looking very simple. In this direction, a problem extremely important in nonequilibrium statistical physics, the relaxation process from nonequilibrium to equilibrium states, has not been (to our knowledge) considered and even the definition of nonequilibrium states for few body mechanical systems has not yet been available.

In statistical physics, there are a number of interesting problems concerning nonequilibrium relaxation processes. The evolution of systems with adiabatic pistons (AP) is among the most conceptionally amazing ones [10–14]. The AP problem considers the relaxation to the equilibrium state with a piston having large mass and forbidding heat flow between its two sides. In this process one may observe a strange phenomenon: as the average piston position moves from right (left) to left (right), one finds energy transport from left (right) to right (left), and this is not intuitively accepted. It has been made clear that this seemingly anti-intuitive phenomenon is caused by the fluctuation of the piston motion [11], which is often ignored in studying relaxation processes of thermodynamic systems. So far, the AP problem has been investigated uniquely for thermodynamic systems having huge numbers of microscopic particles. It is significant if we can study the AP problem in much simpler few-body systems. If we can do so, much more improved understanding could be contributed to this strange and significant nonequilibrium relaxation behavior.

From a mathematical point of view, most of few-body mechanical systems are nonintegrable, they may be mixing, chaotic or may be ergodic in energy surface. It is usually impossible to analytically solve the trajectories of such systems. However, it is possible to solve some of these problems in statistical level (often with reasonable approximations). Analytical results in this direction for any new nontrivial systems will be of much help in understanding physical processes.

In this paper, we will study few-body AP systems, propose a suitable average method to manifest the relaxation processes from nonequilibrium to equilibrium states, and construct a stochastically forced thermodynamic equation to satisfactorily describe the relaxation processes.

II. MODEL AND NONEQUILIBRIUM RELAXATION

Let us start with a few-body AP model, which is supposed to have dynamic structure as simple as possible on one hand and to contain the essential characteristics of the AP problem on the other hand. We consider a piston of mass M, which is adiabatic against heat flow between its two sides. Each side of the piston contains N particles of mass m with $m \ll M$. The particles and the piston move in one-dimensional space of length L, and thus, no penetration through any particle, piston, and boundary is allowed. Free motions are assumed without collision, and all the particle-particle, particle-piston, and particle-boundary collisions are hard and elastic. Therefore, the Hamiltonian of the system reads

$$H = \sum_{i=1}^{N} \frac{p_{il}^2}{2m} + \sum_{j=1}^{N} \frac{p_{jr}^2}{2m} + \frac{p^2}{2M} \tag{1}$$

with p_{il} (p_{jr}) and p being the moments of the ith (jth) particle in the left (right) side and the piston, respectively. It is well known that system (1) is nonintegrable, and not chaotic (all the Lyapunov exponents are zero). Moreover, numerical simulations have shown that this system is mixing and er-

*Corresponding author.

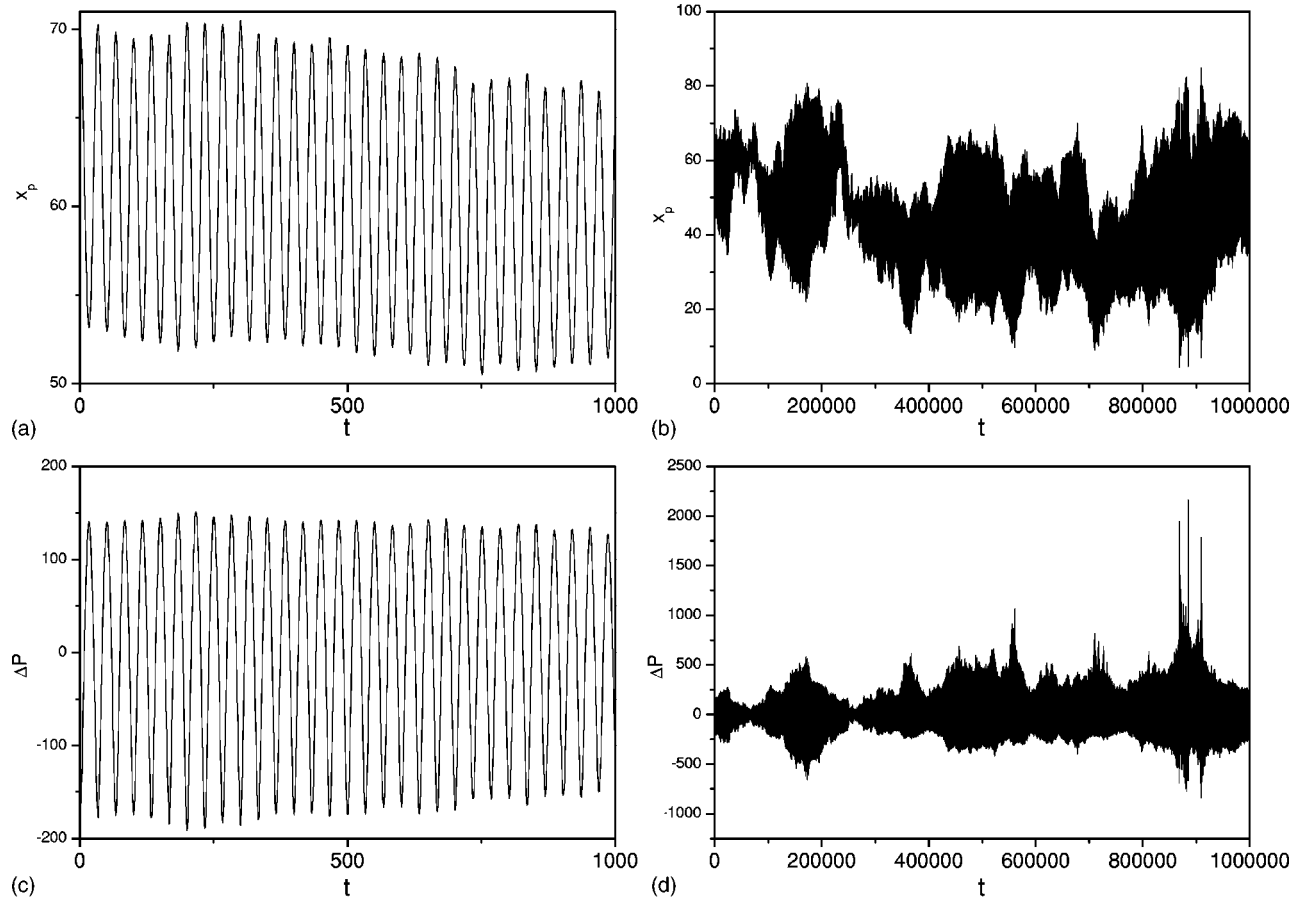

FIG. 1. $m=1$, $M=500$, $N=4$, $v_p=0$, $x_p=70.0$, $E_l(0)=3200$, and $E_r=4000$. These parameters are used in all the following figures except Figs. 4 and 5. $x_i(0)$ and $v_i(0)$ are randomly chosen under the above constraints. (a) $x_p(t)$ plotted vs t for short time scale. (b) $x_p(t)$ vs t for long time scale. (c) Pressure difference $\Delta P(t)=P_l(t)-P_r(t)$ plotted against t for short time scale. (d) $\Delta P(t)$ vs t for long time scale. In (b) and (d), the variations are apparently random and no tendency toward "equilibrium" is observed.

godic in energy surface. Some parameters of (1) can be made irrelevant through scaling. In the following we set

$$m=1, \quad L=100, \quad E_p(0)=0, \quad E=E_l(0)+E_r(0)=7200, \tag{2}$$

where $E_p(0)$, $E_l(0)$ $[E_r(0)]$ are the initial energy of the piston and the energy of all the particles in the left [right] side of the piston, respectively, and E is the total energy of the system. In Fig. 1 we simulate the canonical equations derived from Eq. (1) with $M=500\gg 1$ and a set of arbitrarily chosen initial variables [under condition (2)]. In a short time scale [Fig. 1(a)], we observe oscillatory motion of the piston with a characteristic frequency and slightly random fluctuations in amplitude and phase. In long time scale [Fig. 1(b)], the motion of the piston shows large fluctuation and strong randomness. In Figs. 1(c) and 1(d), and (d) we plot the variation of the pressure difference $\Delta P=P_l-P_r$, where P_l and P_r are pressures of the left and the right sides of the piston, respectively. Numerically, the pressures are measured as

$$P_l=\frac{1}{\Delta t}\left|\sum_{k=1}[mv_l^k(A)-mv_l^k(B)]\right|,$$

$$P_r=\frac{1}{\Delta t}\left|\sum_{k=1}[mv_r^k(A)-mv_r^k(B)]\right|,$$

where the summation includes all collisions $k=1,2,\ldots$ between the piston and the nearest left (for P_l) and right (for P_r) particles, occurring in the time interval of Δt; $v^k(A)$ and $v^k(B)$ represent the velocities of the nearest particle just after and before the kth collision, respectively. Δt is chosen sufficiently small that the piston velocity keeps practically unchanged, while sufficiently large that many collision events happen during Δt. Throughout the paper, we take $\Delta t=1$ for numerical simulations. In Fig. 1(b), one observes that the piston can move towards the central equilibrium position $x_p=L/2$ in certain periods and can move also from the vicinity of $x_p\approx L/2$ to far away in other periods. In Fig. 1(d), the large fluctuation of ΔP indicates as well that the balance between the energies of both sides of the piston is not eventually approached. One can find neither any tendency from nonequilibrium towards equilibrium, nor any characteristic phenomenon of AP systems.

In order to study the relaxations of few-body systems from nonequilibrium states to equilibrium states, the first crucial problem to be solved is how to define few-body in a

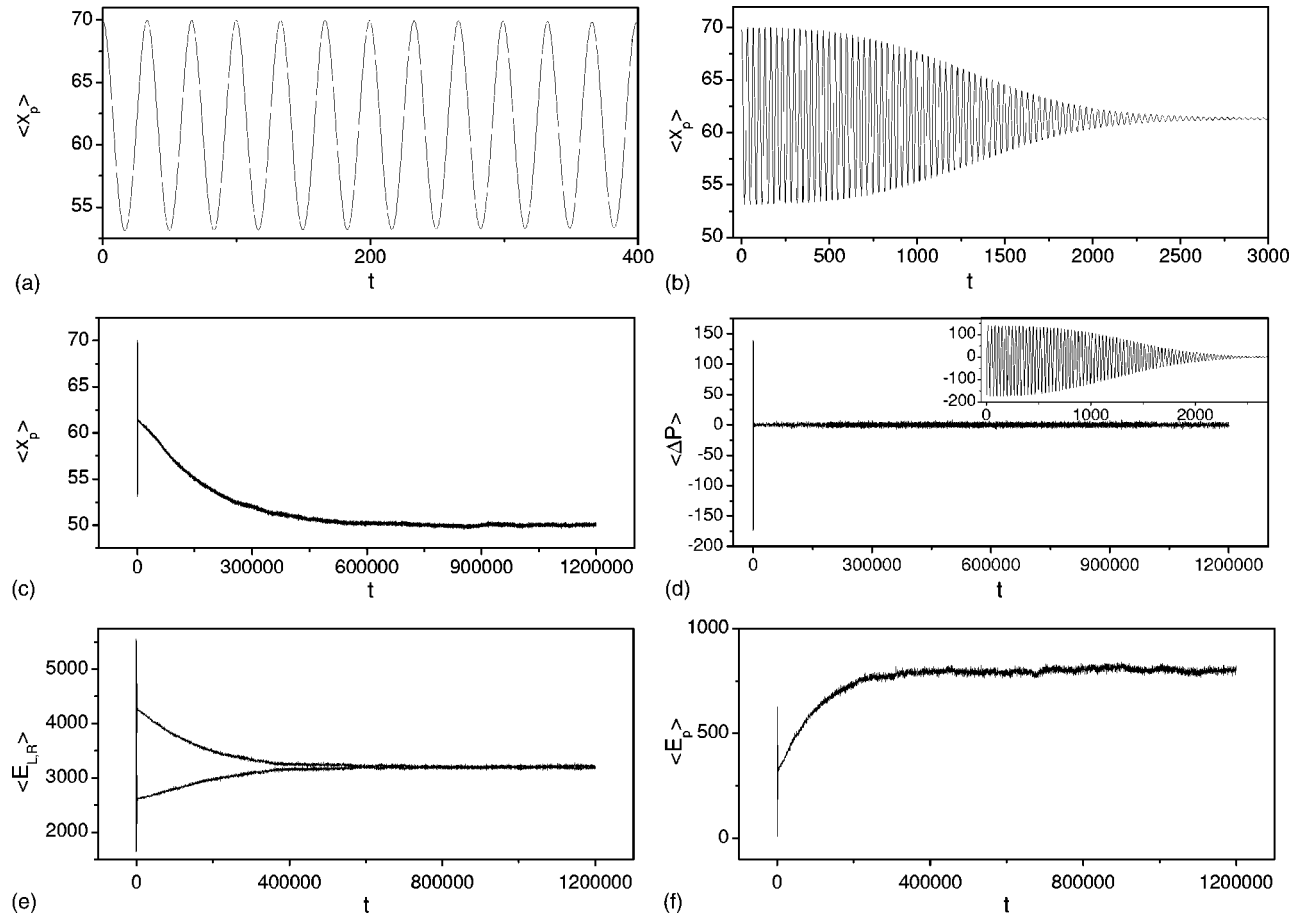

FIG. 2. Data obtained by averaging 10^4 macroscopically identical systems with random initial microscopic variables $x_i(0)$, $v_i(0)$. (a), (b), (c) $\langle x_p(t)\rangle$ plotted vs t for different time scales. Periodic oscillation (a), dissipation of coherence (b), and relaxation to equilibrium (c) are observed in different time stages of the AP evolution. (d) $\langle \Delta P(t)\rangle$ vs t for small (large frame) and large (small frame) time scales. (e) Evolutions of the average particle energies $\langle E_l(t)\rangle$ and $\langle E_r(t)\rangle$. (f) Evolution of the average piston energy. Equal-energy partition $\langle E_l\rangle = \langle E_r\rangle = N\langle E_p\rangle$ is eventually established.

nonequilibrium state. Actually, any few-body state is "nonequilibrium." Equilibrium states of few-body systems have been well defined by long time averages if these systems enjoy ergodicity in energy surfaces [15,16]. However, up to date, there has been no clear definition, to our knowledge, for nonequilibrium of few-body systems because any long time averages give always equilibrium states. For defining nonequilibrium states one has to make ensemble averages (rather than time averages). In our case, we use some slow varying quantities ($E_{l,r}$ and v_p, x_p) for ensemble averages, which are computed for identical initial slow variables and different randomly chosen other fast variables (such as the space positions and the velocities of all small-mass particles).

In Figs. 2(a)–2(d) we do exactly the same as in Fig. 1 with the same initial conditions $E_{l,r}(t=0)$, $v_p(t=0)$, and $x_p(t=0)$. However, unlike a single system with an arbitrarily chosen set of the initial particle variables in Fig. 1, we average all slow quantities in Fig. 2 of 10 000 systems with identical slow variables and different fast variables. Under these ensemble averages, the features of Fig. 2 turn to be dramatically different from those of Fig. 1. Now nonequilibrium and equilibrium states can be defined properly, and relaxations from nonequilibrium to mechanical equilibrium and then to global thermodynamic equilibrium are clearly seen. The characteristic phenomenon of AP systems is demonstrated in our few-body system without any ambiguity.

In Fig. 2 the evolution of the ensemble of systems has three distinctive stages. First, for very small time scale [$t \approx (0,400)$, Figs. 2(a)], we observe well behaved periodic oscillation. This coherent motion is caused by the coherence stored in the initial condition of the slow variables. Second, this coherent oscillation damps for short time scale [$t \approx (400,2500)$, Fig. 2(b)] due to the dissipation caused mainly by the phase diffusion between different systems [this conclusion can be drawn by comparing Figs. 2(a) and 2(b) with Fig. 1(a)]. In the end of the second stage (about $t \approx 2500$), the amplitude of the coherent oscillation damps to nearly zero [Fig. 2(c)] and in the same time the two sides come to mechanical balance $P_l \approx P_r$ [$\Delta P \approx 0$, Fig. 2(d)]; this is exactly what happens in conventional thermodynamic AP systems. The most interesting feature is observed in the third stage when the few-body AP system goes from a mechanically balanced [Fig. 2(d)] while thermally and spatially nonequilibrium state to the globally equilibrium state [$x_p = L/2$ with $E_l = E_r$]. In this stage, the piston monotonously moves to left towards $x_p = L/2$ [Fig. 2(c)] and in the same time one

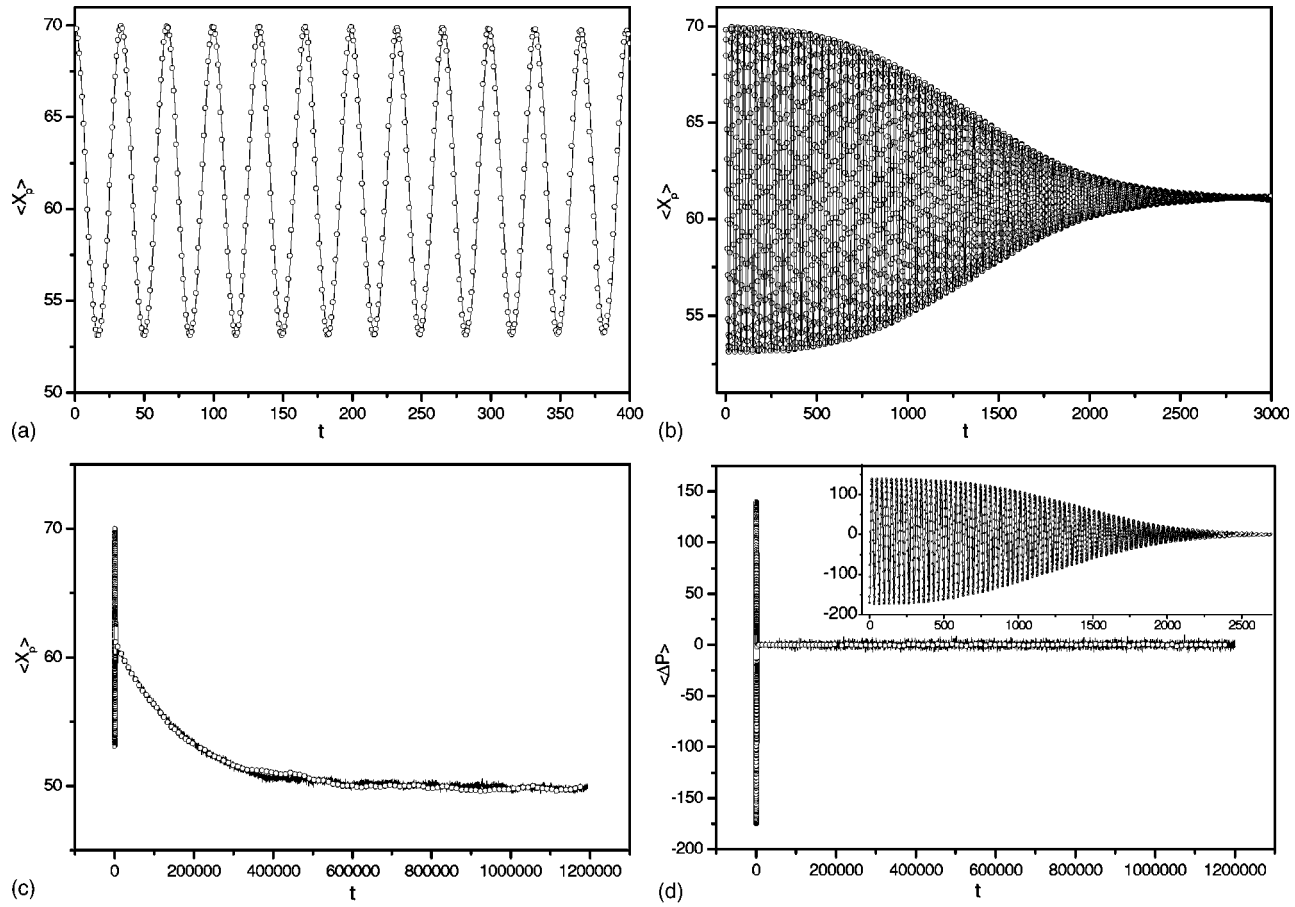

FIG. 3. (a)-(d). Continuous lines: results of Figs. 2(a)–2(d), respectively. Circles: the same as in Figs. 2(a)–2(d), respectively, with data obtained by averaging the results of Eq. (5) with 1000 different noise realizations. Agreements between the theoretical predictions and the direct numerical simulations of the ensemble of the original AP systems are satisfactory.

observes energy transport from the left side to the right side [Fig. 2(e)], and this is a typical AP feature against the intuition. It is interesting to note that at $t \to \infty$ the piston gains energy predicted by the energy-equal partition law $E_p(t \gg 1) \approx E/(2N+1) = 800$ [Fig. 2(f)].

III. STOCHASTICALLY FORCED PHENOMENOLOGICAL EQUATIONS

In Figs. 1 and 2 we demonstrate the dynamic behavior of a single few-body AP system and the averages of an ensemble of such systems, respectively, by purely numerical simulations. Equation (1) is nonintegrable. For any comprehensive analytical understanding one has to seek some approximations based on certain assumptions. Here we adopt the so-called local equilibrium assumption. Since $M \gg m$, the variations of x_p, v_p, and $E_{l,r}$ are much slower than those of x_i and v_i. Therefore, we assume that the left and right particles have sufficiently long time to reach local equilibriums when the piston variables have not been considerably changed. With this assumption, the evolutions of the slow quantities x_p, v_p, and $E_{l,r}$ can be explicitly given as

$$\dot{v}_p = \frac{1}{M}(\overline{P_l} - \overline{P_r}) \tag{3a}$$

$$\dot{\overline{E_l}} = -\overline{P_l} v_p, \quad \dot{\overline{E_r}} = \overline{P_r} v_p \tag{3b}$$

$$\overline{P_l} = \frac{2\overline{E_l}}{x_p}, \quad \overline{P_r} = \frac{2\overline{E_r}}{L - x_p} \tag{3c}$$

We compare the result of direct numerical simulation of the ensemble of systems [Fig. 2(a) or solid line in Fig. 3(a)] with the solution of Eqs. (3) [circles in Fig. 3(a)] for the same initial conditions of $x_p(0)$, $v_p(0)$, and $E_{l,r}(0)$. The theoretical predictions of (3) agree with the numerical results of Eq. (1) perfectly, verifying the validity of the assumption of the local equal-energy partition of Eq. (3c).

Although Eq. (3) can reproduce well the characteristics of the evolution of the average of the ensemble of systems in the very early (the first) time stage, the purely periodic oscillation of Fig. 3(a) cannot explain the dissipative damping in the second stage [Figs. 2(b) and 2(d)] and the anti-intuition feature in the third stage [Figs. 2(c) and 2(d)]. The crucial point ignored in Eqs. (3) is that the pressures $P_{l,r}$ should be subject to inevitable fluctuations. Since particle velocities may quickly lose their memories after few particle-particle and particle-piston collisions, we can simply assume these fluctuations as white noise $\Gamma_{l,r}(t)$

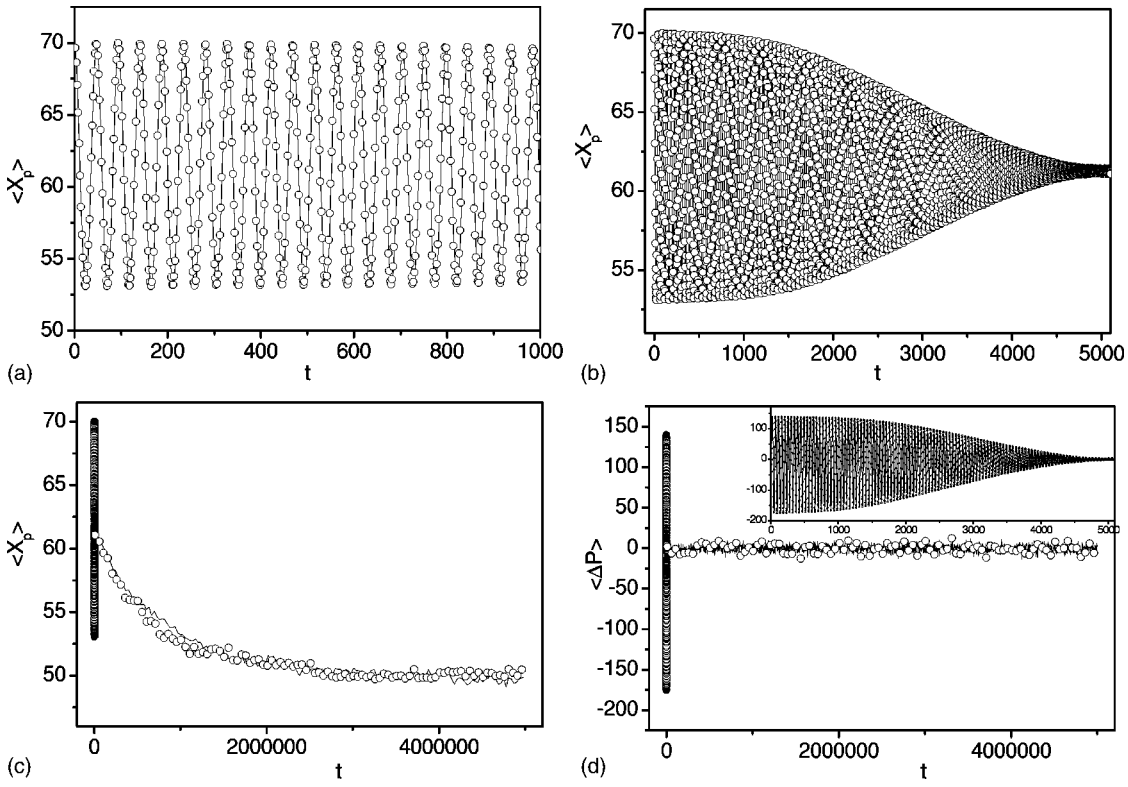

FIG. 4. The same as Fig. 3 with $M=1000$.

$$\frac{P_{l,r}}{M} = \frac{\overline{P_{l,r}}}{M} + \Gamma_{l,r}(t)$$

$$\langle \Gamma_{l,r}(t) \rangle = 0, \tag{4a}$$

$$\langle \Gamma_{l,r}(t)\Gamma_{l,r}(t') \rangle = 2\alpha D_{l,r}\delta(t-t'), \quad \langle \Gamma_l(t)\Gamma_r(t') \rangle = 0,$$

where we set $D_l = E_l/x_p$, and $D_r = E_r/(L-x_p)$, by assuming proportional fluctuations of $P_{l,r}$. According to the fluctuation-dissipation theorem, these fluctuations should be associated with dissipative terms $-\beta_{l,r}v_p$ in Eq. (3a). In addition, the dissipation coefficients $\beta_{l,r}$ are not independent, they are uniquely determined by the fluctuations, based on the Einstein formula of the fluctuation-dissipation theorem [17],

$$\frac{\beta_{l,r}}{\alpha D_{l,r}} = \frac{M}{kT_{l,r}}, \quad kT_{l,r} = \frac{2E_{l,r}}{N},$$

leading to

$$\beta_{l,r} = \frac{\alpha NMD_{l,r}}{2E_{l,r}}. \tag{4b}$$

Equations (4a) and (4b) modify Eq. (3a) to $\dot{v}_p = (1/M)(\overline{P_l} - \overline{P_r}) - (\beta_l + \beta_r)\cdot v_p + \Gamma_l + \Gamma_r$. Since for every action there is an equal and opposite reaction, additional fluctuation and dissipation terms

$$-M\Gamma_{l,r}v_p + M\beta_{l,r}v_p^2$$

should be added to the right-hand side (r.h.s.) of Eqs. (3b) and (3c). Moreover, as $t\to\infty$, the system should go to equilibrium satisfying the equal-energy partition. This requires $\langle v_p \rangle = 0$, $\dot{E}_{l,r} = 0$, $\frac{1}{2}M\langle v_p^2 \rangle = \langle E_l \rangle/N = \langle E_r \rangle N$ for $t\to\infty$. These conditions suggest one more additional terms $-\alpha MD_{l,r}$ in the r.h.s. of Eqs. (3b) and (3c). Finally, Eqs. (3b) and (3c) should be replaced by

$$\dot{E}_l = -\frac{2E_l}{x_p}v_p - \alpha M\frac{E_l}{x_p} - M\Gamma_l \cdot v_p + \frac{\alpha NM^2}{2x_p}\cdot v_p^2 \tag{5a}$$

$$\dot{E}_r = +\frac{2E_r}{L-x_p}\cdot v_p - \alpha M\frac{E_r}{L-x_p} - M\Gamma_r \cdot v_p + \frac{\alpha NM^2}{2(L-x_p)}\cdot v_p^2 \tag{5b}$$

Due to the conservation law of the total energy, the three quantities E_l, E_r, and E_p are not independent. We use Eqs. (5a) and (5b) together with the constraint

$$E = E_p + E_l + E_r \tag{6}$$

for numerical simulations. In Eq. (5) all terms are explicitly and quantitatively given except the parameter α, which we are unable to derive analytically due to the complexity of the few-body systems. Nevertheless, the whole complexity of the nonintegrable and mixing system is now enormously reduced to a single constant, which can be easily determined by numerical fitting.

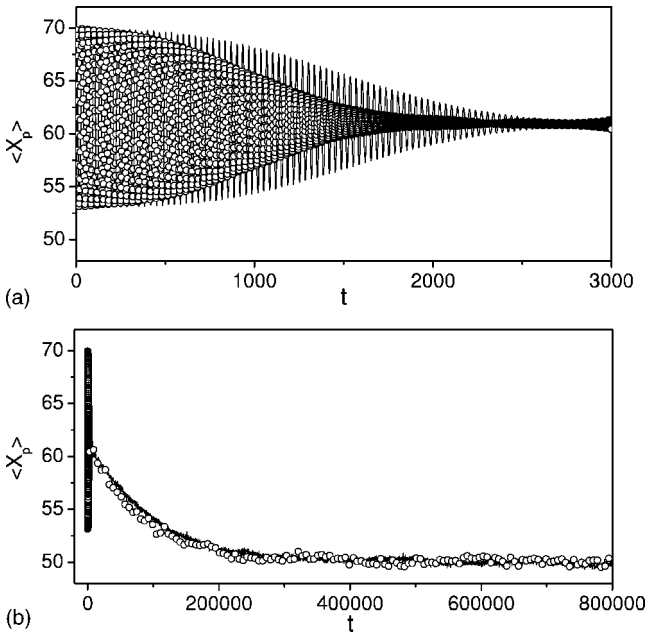

FIG. 5. (a) and (b) The same as Figs. 3(b) and 3(c) with $N=10$. While the qualitative results remain unchanged, obvious quantitative deviations between the theoretical predictions of Eq. (5) (circles) and direct numerical simulations of Eq. (1) (solid lines) are observed for this larger N.

In Figs. 3(a)–3(d) we do the same as in Figs. 2(a)–2(d), respectively, by comparing the results of Eq. (5) (circles) and those of Eq. (1) (continuous lines). All circles plot the data of averages of 1000 different realizations of noises $\Gamma_{l,r}(t)$. It is striking that both evolutions coincide with each other not only qualitatively, but also quantitatively. By adjusting a single parameter α only, we can use Eq. (5) to reproduce satisfactorily the entire evolution from strong nonequilibrium state to partial (mechanical) equilibrium and finally to a global equilibrium state. This agreement shows that the mechanisms implied by the local equilibrium assumption Eq. (3) and the fluctuations of Eqs. (4) and (5) explore the essences of the few-body AP problem, including the periodic coherent oscillation in the first stage, dissipative amplitude damping in the second stage, and the anti-intuition energy transport associated to the relaxation to the global equilibrium in the third stage. As $t\to\infty$ the equal-energy partition is asymptotically established by Eqs. (5), i.e., we observe $\langle E_l(t\to\infty)\rangle = \langle E_r(t\to\infty)\rangle \to 3200$, and $\langle E_p(t\to\infty)\rangle \to 800$ eventually. It is emphasized that the inclusion of fluctuations is the key point for the success of Eq. (5).

Equation (5) is valid approximately for arbitrary $N(N\geqslant 1)$ and $M(M\gg m)$; the validity is well confirmed by numerical simulations. In Fig. 4 we do exactly the same as in Fig. 3 for $M=1000$; the results are the same as for Fig. 3 except that the time scale of evolution is enlarged. In Figs. 5(a) and 5(b) we do the same as in Fig. 3(b) and 3(c), respectively, by taking $N=10$ and $M=500$. Both the direct numerical simulations (solid lines) and the stochastically phenomenological equations (circles) show behaviors similar to those of Fig. 3. Quantitatively, deviations between the solid lines and the dots are, however, observed clearly. The reason is that for larger N, the system needs a longer relaxation time to reach local equal-energy partition, and the assumption of a local equal-energy partition is no longer valid in the piston motion. We find that for larger N, the local equal-energy partition and also the agreement between the numerical results and theoretical prediction can be improved by increasing the ratio M/m (i.e., by slowing down the motion of the heavy piston). However, for considerably larger M/m the relaxation becomes extremely slow, and the corresponding numerical simulation turns to be extremely time consuming. We will not go further in this direction.

The results of Fig. 5 can be used to explain why all previous numerical simulations of AP systems did not agree quantitatively with theoretical predictions (e.g., see [11,12]). All analytical computations of thermodynamic AP systems performed so far have been based on local equilibrium assumption (namely, local Boltzmann distribution of particle velocities and local equal-energy partitions). For a thermodynamic system with a huge number of particles this assumption can be approximately valid only if the ratio of the piston mass over the particle mass M/m is huge. However, for huge M/m the relaxation of the AP system is extremely slow and is impractical for actual numerical simulations. For realistic numerical simulations one often uses parameters $N\approx 10^2-10^3$ with $M/m\approx 10^2-10^3$, at which the deviation from local equilibrium is large and thus the numerical results obtained in these ranges of parameters are certainly not in agreement with the theoretical predictions ([11,12]). It is then remarkable that with few-particle AP systems, agreement between direct numerical simulations and theoretical predictions of stochastic phenomenological equations can be easily achieved, and the mechanism underlying the interesting characteristics of the AP systems can be demonstrated in a more apparent manner.

IV. CONCLUSION

In conclusion, we have suggested a nonintegrable and mixing few-particle model with a heavy piston, which shows random motion for its long time evolution. With proper ensemble averages, we observe coherent oscillation with characteristic frequency, regular dissipative damping of oscillation amplitude, directional relaxation from nonequilibrium to equilibrium state, and the anti-intuition energy transport of the adiabatic piston in this relaxation. All these interesting features are explained and reproduced by a noise-driven Eq. (5) that is derived from the assumptions of local equilibrium thermodynamics and fluctuations in this thermodynamics. It is emphasized that all theoretical assumptions are based on some phenomenological considerations based on certain physical reasoning. Numerical simulations approximately verify the validity of the analysis.

So far, the problem of relaxation of nonequilibrium systems has been defined and investigated uniquely for macroscopic systems consisting of huge numbers of subsystems (say, particles). Here, with a proper classification of slow and fast variables, we convincingly show relaxation from nonequilibrium to equilibrium with ensemble average of many

few-particle systems having identical initial slow variables. We hope the results and the approaches in this paper may stimulate new investigations of nonequilibrium states of few-body nonintegrable and chaotic systems, and also novel studies of few-body adiabatic piston problems.

ACKNOWLEDGMENTS

This work was supported by the National Natural Science Foundation of China under Grant Nos. 10335010 and 10175010 and by the Nonlinear Science Project.

[1] G. Casati, J. Ford, F. Vivaldi, and W. M. Visscher, Phys. Rev. Lett. **52**, 1861 (1984).
[2] Ya. G. Sinai, *Ergodic Theory with Applications to Dynamical Systems and Statistical Mechanics Systems II* (Springer-Verlag, Berlin, 1989).
[3] G. J. Ackland, Phys. Rev. E **47**, 3268 (1993).
[4] E. Ott, *Chaos in Dynamical Systems* (Cambridge University Press, Cambridge, UK, 1993).
[5] Z. Zheng, G. Hu, and J. Zhang, Phys. Rev. E **52**, 3440 (1995).
[6] Z. Zheng, G. Hu, and J. Zhang, Phys. Rev. E **53**, 3246 (1996).
[7] S. Sasa and T. S. Komatsu, Phys. Rev. Lett. **82**, 912 (1999).
[8] S. G. Cox and G. J. Ackland, Phys. Rev. Lett. **84**, 2362 (2000).
[9] H. Li, Z. Cao, and G. Hu, Phys. Rev. E **67**, 041102 (2003).
[10] R. P. Feynman, *The Feynman Lectures on Physics I* (Caltech, 1965), chap. 39.
[11] J. Piasecki and Ch. Grüber, Physica A **265**, 463 (1999); Ch. Grüber and J. Piasecki, *ibid.* **268**, 412 (1999).
[12] E. Kestemont, C. V. Broeck, and M. M. Mansour, Europhys. Lett. **49**, 143 (2000).
[13] J. A. White, F. L. Román, A. González, and S. Velasco, Europhys. Lett. **59**, 479 (2002).
[14] T. Munakata and H. Ogawa, Phys. Rev. E **64**, 036119 (2001).
[15] V. L. Berdichevsky, J. Appl. Math. Mech. **52**, 738 (1988).
[16] V. L. Berdichevsky and M. V. Alberti, Phys. Rev. A **44**, 858 (1991).
[17] H. Risken, *The Fokker-Planck Equation* (Springer-Verlag, Berlin, 1984).