Piston dynamics from a microcanonical ensemble

Masayuki Uranagase and Toyonori Munakata
Department of Applied Mathematics and Physics, Graduate School of Informatics, Kyoto University, Kyoto 606-8501, Japan
(Received 14 March 2006; published 12 January 2007)

The dynamical behavior of a system consisting of a (heavy) piston and two rectangular boxes, each containing two hard disks and in contact with the piston, is studied based on a projection operator method for a microcanonical ensemble. We derive a coupled set of nonlinear equations for slow variables of the system and solve it to confirm that our theory with no adjustable parameters reproduces experimental results fairly well. Some limitations of the theory are discussed from the viewpoint of the separation of slow and fast time scales and ergodicity.

DOI: 10.1103/PhysRevE.75.011110 PACS number(s): 05.20.Jj, 05.20.Gg, 05.45.Ac

I. INTRODUCTION

The dynamics of an adiabatic piston offers interesting problems [1,2], and recently it has gathered a lot of attention in connection with both fundamentals and applications of statistical mechanics. One considers that a cylinder with finite or infinite length is separated into two compartments by a piston and each compartment is filled with gas particles. It is supposed that the mass of the piston, M, is much larger than that of a gas particle, m. Initially the piston is fixed by a brake and the gas in the left (right) compartment is kept in thermal equilibrium with the pressure p_L (p_R) and the temperature T_L (T_R). At a certain time, a brake is released and our interest is in relaxation of the whole system, the piston and gases, toward a total equilibrium state. This problem was recently investigated by using various methods for various gases, typically consisting of ideal (noninteracting) or hard-core (or disk) particles. The Boltzmann equation [3,4] and master equation [5,6] are employed for a piston interacting with an ideal gas and hydrodynamic equation [7,8] and molecular dynamics simulations [9] are employed to study the dynamics of a piston in hard disks.

In the case where the length of the cylinder is infinite with $p_L=p_R$ and $T_L\neq T_R$, the piston stationarily moves to a hotter region. A stationary velocity of the piston can be obtained from analysis of the Boltzmann equation [3,4]. This phenomenon can also be explained by other approaches. For instance, a Fokker-Planck equation for the velocity V of the piston has a stationary solution of the form $\propto \exp[-\Phi_{st}(V)]$ and the stationary velocity of the piston $V_{st}\propto\int V\exp[-\Phi_{st}(V)]dV$ is not equal to 0 [5].

On the other hand, in the case where the length of the cylinder is finite, relaxation to an equilibrium state is characterized by two stages. The first stage is relaxation to a mechanical equilibrium state, where $p_L=p_R$ and $T_L\neq T_R$ [7,8,10]. In this process, molecular dynamics simulation shows that the dynamics of the piston exhibits damped oscillatory motion. This motion is predicted for the piston in contact with an ideal gas from a Liouville equation [10]. It also comes from a hydrodynamic approach [7,8]. The second stage, which is much slower than the first one, is relaxation to thermal equilibrium of the whole system, where not only $p_L=p_R$ but also $T_L=T_R$. In this process, it is confirmed numerically and theoretically that the piston moves to a hotter region and conducts heat [9,11]. For a system consisting of a piston and two hard-disk gases, one can see that the power spectral density of the system in the total equilibrium state has three peeks: i.e., two damped sound modes related to oscillatory motion and a thermal mode related to slow relaxation at the second stage [12].

It is also possible to derive an equation of motion, which describes oscillatory behavior of a piston in a potential field, in a system of finitely many noninteracting [13]. In the derivation collisions between the piston and gas particles during a time interval $\delta\sqrt{M/k_BT}$, with δ and k_B denoting some displacement of the piston and Boltzmann constant, respectively, are considered and the limit $\delta\to 0$ is taken after $M\to\infty$. For the case of interacting gas particles, a similar equation of motion is also obtained by using an averaging method [14].

In most of the studies of the adiabatic piston problem, each compartment contains many gas particles. However, it is of interest to consider the case where each compartment has a few particles since it can have close relations with the foundation of statistical mechanics [15], equilibrium statistical mechanical properties [16], and some dynamical properties [17–19]. In this paper we consider a two-dimensional rectangular box, which is separated by a piston into two boxes each containing two hard disks. For a rectangular box with two or three hard disks, the microcanonical partition function, denoted by Z_{RB}, is calculated exactly [20,21]. It is noted that the pressure p calculated from Z_{RB} has been compared with the time-averaged pressure $\bar{p}$ obtained from molecular dynamics simulations [20,21] and $p=\bar{p}$ has been confirmed as a partial check on ergodicity of the system.

The fact that an exact partition function Z for our piston problem is available also offers an interesting opportunity to study dynamical behaviors such as relaxation of the system [11,19], and we pursue this possibility for our system. Under the assumption that the phase-space distribution function quickly or more precisely instantaneously relaxes to a nonequilibrium microcanonical distribution characterized by a set of slow variables—say, a—i.e., a quasiequilibrium assumption—we derive a Fokker-Planck equation for the slow variables by applying a projection operator method. This Fokker-Planck equation is dependent on the equilibrium distribution function of fast variables which is obtained from Z. Moreover, we derive a set of nonlinear equations for slow

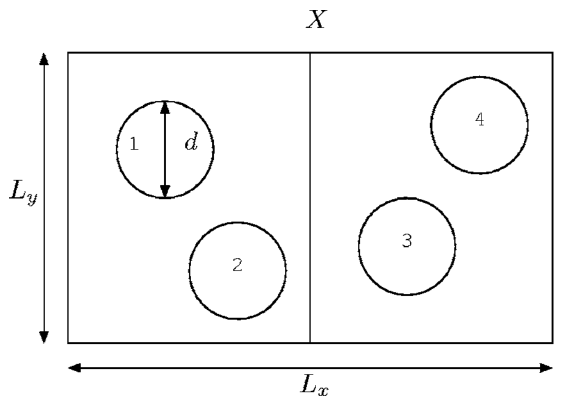

FIG. 1. A piston and two rectangular boxes, each containing two hard disks. The piston at X with momentum P can slide only along the x direction.

variables from the Fokker-Planck equation and confirm that these equations with energy conservation law reproduce results obtained from molecular dynamics simulations fairly well.

At this point it is worthwhile to note that a quasi equilibrium assumption naturally leads to neglect of some dynamical correlations and our theory is approximate [17] even if an exact Z is available for a system. This situation is similar to the one in the Boltzmann equation, which is approximate due to the introduction of the hypothesis of molecular chaos, even if one knows exact form for a differential cross section.

This paper is organized as follows. First we introduce the model studied in this paper and investigate its equilibrium properties under a microcanonical ensemble in Sec. II. In Sec. III, we derive a Fokker-Planck equation for slow variables by using a projection operator method and a quasi equilibrium assumption. Finally, in Sec. IV, we derive a set of nonlinear equations from the Fokker-Planck equation by neglecting a diffusion (or conduction) part. The nonlinear equations are solved numerically to compare with molecular dynamics simulations. The final section contains discussions of the dynamics of the piston based on a mass-ratio expansion and conclusions.

II. MODEL AND ITS EQUILIBRIUM PROPERTIES

The system which we study in this paper is depicted in Fig. 1. The box with size L_x and L_y contains a piston with mass M which separates the box into two boxes each with two hard disks inside. We denote momentum and position of the particle i $(=1,\ldots,4)$ by $\hat{\boldsymbol{p}}_i$ and $\hat{\boldsymbol{r}}_i$, respectively. Here it is remarked that $\hat{\boldsymbol{p}}_i$ means that it is a dynamical variable and $\boldsymbol{p}_i$ is used to denote its value. The piston with momentum $\hat{P}$ and position $\hat{X}$ can slide in the x direction. The Hamiltonian of the system is thus

$$\hat{H} = \sum_{i=1,2} \frac{\hat{\boldsymbol{p}}_i^{\,2}}{2m} + \sum_{i=3,4} \frac{\hat{\boldsymbol{p}}_i^{\,2}}{2m} + \frac{\hat{P}^2}{2M} \equiv \hat{H}_L + \hat{H}_R + \hat{H}_P. \tag{1}$$

When $m \ll M$ it is considered that the set of variables $\hat{a} \equiv (\hat{P},\hat{X},\hat{H}_L,\hat{H}_R)$ changes in time slowly compared with other variables such as $\hat{\boldsymbol{p}}_i$ and we introduce a microscopic density

$$\hat{D}(a,t;\Gamma) \equiv \delta(\hat{a}(t;\Gamma) - a) = \delta(\hat{P}(t) - P)\,\delta(\hat{X}(t) - X)\,\delta(\hat{H}_L(t) - H_L)\,\delta(\hat{H}_R(t) - H_R).$$

where Γ represents a point in the 18-dimensional phase space. Here $\hat{a}(t;\Gamma)$ means that this is a function of both time t and an initial phase Γ, similar to Heisenberg representation in quantum mechanics. This point is detailed in the Appendix.

First we consider for later convenience the equilibrium distribution of a, which is given by a microcanonical ensemble average of the microscopic density $\hat{D}(a,t=0;\Gamma) \equiv \hat{D}(a;\Gamma)$—i.e., $D_{eq}(a)=\{Z(H)\}^{-1}\int d\Gamma \hat{D}(a;\Gamma)\,\delta(\hat{H}-H) \equiv \langle \delta(\hat{H}-H)\rangle$ with $Z(H)=\int d\Gamma\, \delta(\hat{H}-H)$. Denoting the (configurational) partition function of the two hard disks in a box of size (l_x,l_y) by $Z_2(l_x,l_y)$ [20], we have

$$D_{eq}(a) = f_{eq}(X) f_{eq}(P,H_L,H_R), \tag{2}$$

with [22]

$$f_{eq}(X) = \frac{Z_2(X,L_y)Z_2(L_x - X,L_y)}{Z_c}. \tag{3}$$

Here Z_c is a normalization to ensure $\int dX f_{eq}(X)=1$.

The piston momentum distribution $f_{eq}(P)=\int dH_L dH_R \times f_{eq}(P,H_L,H_R)$ is simply given by

$$f_{eq}(P) = \frac{(2mH - P^2)^3}{\displaystyle\int dP(2mH - P^2)^3}, \tag{4}$$

where the integration in Eq. (4) is limited to the region $(2mH-P^2)\geqslant 0$. The distribution of the momentum p_x of a hard disk—say, $i=1$—when $\hat{H}_L=H_L$ is similarly obtained as

$$f_{eq}(p_x|H_L) = \frac{(2mH_L - [p_x]^2)^{1/2}}{(m\pi H_L)}. \tag{5}$$

In Fig. 2, we compare Eqs. (3) and (4) with molecular dynamics simulations—i.e., long time average. In this paper, as units of length and mass, the diameter d and mass m of a hard disk are chosen, respectively, and the system in Fig. 2 is characterized by $H=18$, $M=100$, $L_x=15$, and $L_y=3$.

Agreement between these distribution functions from the microcanonical ensemble and molecular dynamics simulations gives partial support to the ergodicity of our system. Equipartition laws—i.e., $\langle \hat{P}^2/(2M)\rangle = H/9$ and $\langle \hat{p}_x^2/(2m)\rangle = H_L/4$—readily follow from Eqs. (4) and (5).

III. PROJECTION OPERATOR METHOD FOR PISTON DYNAMICS

With use of a projection operator method [23,24] (see the Appendix), one can rewrite the equation of motion for $\hat{D}(a,t;\Gamma)$ in an exact form

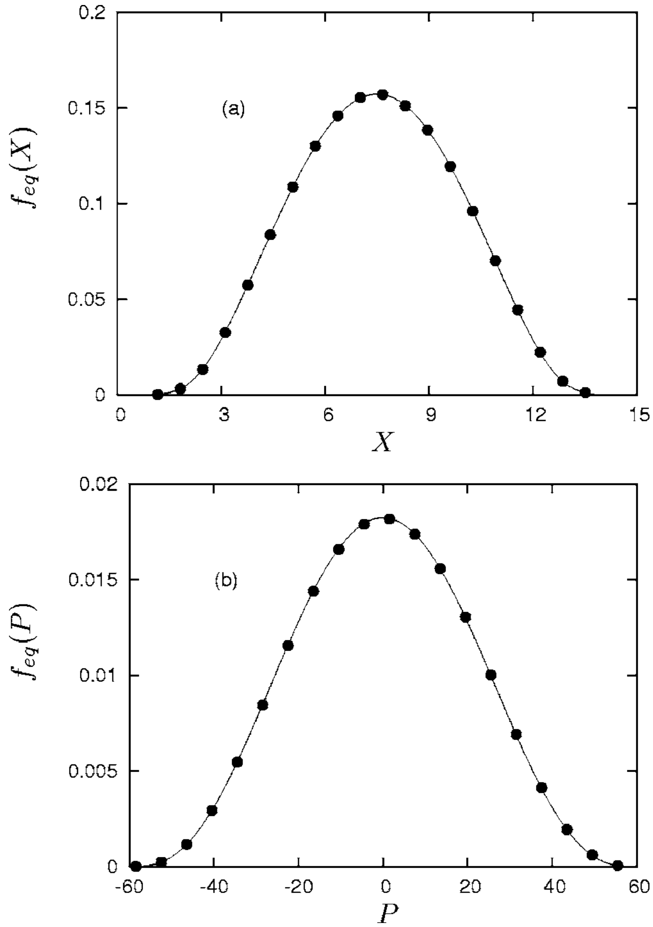

FIG. 2. Distribution functions of (a) X and (b) P. Theoretical predictions based on Eqs. (3) and (4) and numerical results from molecular dynamics experiments are plotted by solid curves and solid circles, respectively. Parameters are chosen as $H=18$, $M=100$, $L_x=15$, and $L_y=3$.

$$\frac{\partial \hat{D}(a,t;\Gamma)}{\partial t} = \int da'\,\Omega(a,a')\hat{D}(a',t;\Gamma) - \int da' \int_0^t ds\,\phi(a,a',t-s)\hat{D}(a',s;\Gamma) + \hat{N}(a,t), \tag{6}$$

where $\int da'$ means integration over the four macrovariables and Eq. (6) is obtained by setting $\hat{A}_i(t)$ equal to $\delta(\hat{a}(t;\Gamma)-a)$ in Eq. (A13).

From Eqs. (A3) and (A11), the frequency matrix $\Omega(a,a')$ and the damping matrix $\phi(a,a',t)$ are written as follows:

$$\Omega(a,a') = \int da'' \langle L\hat{D}(a;\Gamma),\hat{D}(a'';\Gamma)\rangle \langle \hat{D},\hat{D}\rangle^{-1}(a'',a'), \tag{7}$$

$$\phi(a,a',t) = \int da'' \langle \hat{N}(a,t),\hat{N}(a'')\rangle \langle \hat{D},\hat{D}\rangle^{-1}(a'',a'). \tag{8}$$

Here $\langle \hat{A},\hat{B}\rangle$ denotes a microcanonical ensemble average of $\hat{A}\hat{B}$, $\langle \hat{A}\hat{B}\rangle$, $\hat{D}(a;\Gamma)\equiv\hat{D}(a,t=0;\Gamma)$, and $L\hat{D}(a;\Gamma) \equiv (\partial\hat{D}(a,t;\Gamma)/\partial t)|_{t=0}$. The random "force" $\hat{N}(a)\equiv\hat{N}(a,t=0)$ is defined by Eq. (A7) [23,24]:

$$\hat{N}(a) = \left.\frac{\partial \hat{D}(a,t;\Gamma)}{\partial t}\right|_{t=0} - \int da'\,\Omega(a,a')\hat{D}(a';\Gamma) \equiv (1-\mathcal{P})L\hat{D}(a;\Gamma). \tag{9}$$

The projection operator $\mathcal{P}$ projects an arbitrary variable onto the space whose element is expressed as a linear combination of $\hat{D}(a;\Gamma)$ in the form $\int da' Q(a')\hat{D}(a';\Gamma)$ with $Q(a)$ denoting a linear coefficient which is a function of a. Finally we note that $\hat{N}(a,t)$ evolves in time through a modified propagator $\exp[(1-\mathcal{P})Lt]$ instead of the natural one, $\exp[Lt]$.

Let us calculate $\Omega(a,a')$ and $\phi(a,a',t)$ following the definitions (7) and (8). Calculations are mostly trivial, and only some aspects including (elastic) collisions will be touched upon. From the relation

$$L\hat{D}(a;\Gamma) = -\frac{\hat{P}}{M}\nabla_X\hat{D}(a;\Gamma) - \hat{F}\nabla_P\hat{D}(a;\Gamma) - \hat{W}_L\nabla_{H_L}\hat{D}(a;\Gamma) - \hat{W}_R\nabla_{H_R}\hat{D}(a;\Gamma) \equiv \hat{C}_1+\hat{C}_2+\hat{C}_3+\hat{C}_4, \tag{10}$$

with $\hat{F}\equiv d\hat{P}/dt$, $\hat{W}_L\equiv d\hat{H}_L/dt$, and $\hat{W}_R\equiv d\hat{H}_R/dt$, it is evident that $\Omega(a,a')$ consists of four contributions, each coming from $\hat{C}_i(i=1,\ldots,4)$. $\hat{C}_1$ is seen to give

$$\left[\int da'\,\Omega(a,a')\hat{D}(a';\Gamma)\right]_1 = -\frac{P}{M}\nabla_X\hat{D}(a;\Gamma). \tag{11}$$

The contribution of $\hat{C}_2$ is obtained by first expressing the time derivative $d\hat{P}/dt$ by $\Delta P/\Delta t=(2M\hat{p}_x-2m\hat{P})/[(m+M)\Delta t]$ where a collision between the piston with momentum P and a hard disk with momentum p_x in time Δt is considered. Since a piston can collide with a hard disk on both sides of the piston, we have

$$\left[\int da'\,\Omega(a,a')\hat{D}(a';\Gamma)\right]_2 = -\nabla_P\hat{D}(a;\Gamma)[F_L(a)+F_R(a)], \tag{12}$$

with

$$F_L(a) = \frac{2mM\rho_L(X-d/2)}{m+M}\int_L dp_x\left(\frac{p_x}{m}-\frac{P}{M}\right)^2 f_{eq}(p_x|H_L) \tag{13}$$

and $F_R(a)$ is similarly defined. $F_L(a)$ denotes an average force on the piston due to collisions with hard disks in the left box. $\rho_L(x)(d/2<x<X-d/2)$ denotes the (one-dimensional) hard-disk density, and $\rho_L(X-d/2)$ is the contact

density with the piston. $\int_{L(R)}$ means that the range of p_x is limited to $(p_x/m-P/M)\geqslant 0(\leqslant 0)$.

$\rho_L(X-d/2)$ is generally related to the pressure $p_L(X,H_L)$ by [25]

$$p_L(X,H_L)=T_L\rho_L\left(X-\frac{d}{2}\right), \tag{14}$$

with $T_L\equiv H_L/2$. Since $p_L(X,H_L)$ is given by

$$p_L(X,H_L)=T_L\frac{\partial \ln Z_2(X,L_y)}{\partial X}, \tag{15}$$

we obtain

$$\rho_L(X-d/2)=\frac{\partial \ln Z_2(X,L_y)}{\partial X}. \tag{16}$$

$\rho_L(x)$ and $\rho_R(x)(X+d/2<x<L_x-d/2)$ are spatially inhomogeneous [20], highest at the wall.

The contribution from $\hat{C}_3$ and $\hat{C}_4$ can be similarly calculated. Thus we express $d\hat{H}_L/dt$ as $\Delta\hat{H}_L/\Delta t$ with $\Delta\hat{H}_L=2[Mp_x^2+(M-m)p_xP-mP^2]/(M+m)^2$ denoting the increment of the piston's kinetic energy due to collision with a hard disk. Taking into account the collision frequency as we did in deriving Eq. (13), we have

$$\left[\int da'\Omega(a,a')\hat{D}(a';\Gamma)\right]_{3+4}=-\nabla_{H_L}\hat{D}(a;\Gamma)W_L(a)-\nabla_{H_R}\hat{D}(a;\Gamma)W_R(a), \tag{17}$$

with

$$W_L(a)=\frac{2\rho_L(X-d/2)}{(m+M)^2}\int_L dp_x[-Mp_x^2-(M-m)p_xP+mP^2]\times\left(\frac{p_x}{m}-\frac{P}{M}\right)f_{eq}(p_x|H_L) \tag{18}$$

being an average rate of change of $\hat{H}_L$ due to collision with the piston. A similar expression holds for $W_R(a)$.

Now we turn to the damping matrix $\phi(a,a',t)$, Eq. (8), which is to be neglected in numerical computations in the next section. First we note that the noise $\hat{N}(a)$ is expressed from Eqs. (9), (11), (12), and (17) as

$$\begin{aligned}\hat{N}(a)&=-\nabla_P\hat{D}(a;\Gamma)[\hat{F}-F_R(a)-F_L(a)]\\&\quad-\nabla_{H_L}\hat{D}(a;\Gamma)[\hat{W}_L-W_L(a)]\\&\quad-\nabla_{H_R}\hat{D}(a;\Gamma)[\hat{W}_R-W_R(a)]\\&\equiv\hat{A}_1+\hat{A}_2+\hat{A}_3.\end{aligned} \tag{19}$$

If we neglect cross correlation functions such as $\langle\hat{A}_1(t)\hat{A}_2(0)\rangle$, which naturally occurs in Eq. (A11), and correlations between successive collisions between the piston and a hard disk (assumption of molecular chaos), we can show that A_1 gives rise to

$$\left[\int da'\int_0^t ds\phi(a,a',t-s)\hat{D}(a',s;\Gamma)\right]_1=-\nabla_P\zeta_P(a)D_{eq}(a)\nabla_P\left[\frac{\hat{D}(a,t;\Gamma)}{D_{eq}(a)}\right]\equiv\hat{B}_1, \tag{20}$$

with

$$\zeta_P(a)=\left(\frac{2mM}{m+M}\right)^2\left\{\rho_L\left(X-\frac{d}{2}\right)\int_L dp_x\left(\frac{p_x}{m}-\frac{P}{M}\right)^3 f_{eq}(p_x|H_L)+\rho_L\left(X+\frac{d}{2}\right)\int_R dp_x\left(\frac{P}{M}-\frac{p_x}{m}\right)^3 f_{eq}(p_x|H_R)\right\}. \tag{21}$$

Similarly we see that

$$\begin{aligned}\left[\int da'\int_0^t ds\phi(a,a',t-s)\hat{D}(a',s;\Gamma)\right]_{2+3}&=-\nabla_{H_L}\zeta_{H_L}(a)D_{eq}(a)\nabla_{H_L}\left[\frac{\hat{D}(a,t;\Gamma)}{D_{eq}(a)}\right]\\&\quad-\nabla_{H_R}\zeta_{H_R}(a)D_{eq}(a)\nabla_{H_R}\left[\frac{\hat{D}(a,t;\Gamma)}{D_{eq}(a)}\right]\equiv\hat{B}_2+\hat{B}_3,\end{aligned} \tag{22}$$

with

$$\zeta_{H_L}(a)=\rho_L\left(X-\frac{d}{2}\right)\left(\frac{2}{m+M}\right)^2\int_L dp_x\times(mP^2-(M-m)p_xP-Mp_x^2)^2\left(\frac{p_x}{m}-\frac{P}{M}\right)f_{eq}(p_x|H_L) \tag{23}$$

and a similar expression for $\zeta_{H_R}(a)$.

If Eq. (6) is averaged over an initial distribution $f(\Gamma,t=0)$ in the Γ space, which depends on Γ only through $\hat{a}$, one can safely neglect the noise $\hat{N}(a,t)$ [23,24] in Eq. (6) and we finally arrive at, with $D(a,t)=\int d\Gamma\hat{D}(a,t;\Gamma)f(\Gamma,t=0)$,

$$\frac{\partial D(a,t)}{\partial t}=\left[-\frac{P}{M}\nabla_X-\nabla_P[F_L(a)+F_R(a)]-\nabla_{H_L}W_L(a)-\nabla_{H_R}W_R\right]D(a,t)+B_1+B_2+B_3, \tag{24}$$

where $\hat{D}(a,t;\Gamma)$ in Eqs. (20) and (22) is replaced by $D(a,t)$ in B_i $(i=1,2,3)$ in Eq. (24).

The Fokker-Planck equation (24) [26] consists of terms with first-order differential operators, representing streaming terms coming from the frequency matrix $\Omega(a,a')$, Eq. (7), and terms with second-order differential operators in $B_1+B_2+B_3$ coming from the damping matrix, Eq. (8). It is noted that our $\Omega(a,a')$ given above is exact. On the other hand, to calculate $\phi(a,a',t)$ we neglected cross-correlation functions and dynamical correlations resulting from successive collisions among the piston, the hard disks, and walls.

Since the damping coefficients $\zeta_P(a)$, Eq. (21), $\zeta_{H_{L(R)}}$, Eq. (23), and the equilibrium distribution function $D_{eq}(a)$, Eq. (2), are complicated functions of a, solving the Fokker-Planck equation, a partial differential equation with 5 space-time variables numerically is beyond our ability. Also it is noted that even if we contend ourselves by solving some (lower-order) moment equations derived from the Fokker-Planck equation, like the 13-moment method by Grad for the Boltzmann equation [27], we still cannot obtain a closed set of equations without introducing serious approximations, which obscures what we do to analyze the Fokker-Planck equation. From these we will simply neglect the second-order diffusion part of the Fokker-Planck equation and solve the first-order partial differential equation, which is equivalent, as is well known, to a (generally nonlinear) set of differential equations for a.

IV. RESULTS AND DISCUSSIONS

Based on the remark given at the end of the previous section, we consider the following set of ordinary differential equations:

$$\frac{dX(t)}{dt} = \frac{P}{M}, \tag{25}$$

$$\frac{dP(t)}{dt} = F_L(a) + F_R(a), \tag{26}$$

$$\frac{dH_L}{dt} = W_L(a), \quad \frac{dH_R}{dt} = W_R(a). \tag{27}$$

The set of equations (25)–(27) is highly nonlinear, and we have solved it numerically. At this point we note that this set of equations does not satisfy the conservation of energy $d[P^2/(2M)+H_L+H_R]/dt=0$. In our studies on relaxation to equilibrium, a similar situation was encountered and we follow the same procedure employed in [19]. That is, to determine X, P, H_L, and H_R as functions of t we always use Eqs. (25) and (26) and $[P^2/(2M)+H_L+H_R]=H$. We need one more equation, for which we employ the first one and the second one of Eq. (27) alternatively.

For molecular dynamics experiments, the initial conditions of $\hat{\boldsymbol{r}}_i(0)$ $(i=1,\ldots,4)$ are chosen from uniformly distributed random numbers. In the process of preparing the initial conditions, if a certain disk—say, $i=2$—overlaps the disk $i=1$, then we choose $\hat{\boldsymbol{r}}_2(0)$ again by the same method until no overlapping is achieved. The α ($\alpha=x$ or y) component of $\hat{\boldsymbol{p}}_i(0)$ $(i=1,2)$ is put as $K_L u_{i,\alpha}$, where $u_{i,\alpha}$ is a random number distributed uniformly between -1 and 1, and K_L is chosen to satisfy the initial condition $H_L=K_L^2\Sigma_i(u_{i,x}^2+u_{i,y}^2)/2m$. Similarly we choose $\hat{\boldsymbol{p}}_i(0)$ $(i=3,4)$.

In Fig. 3 we depict $X(t)$ in a short [Fig. 3(a)] and a long [Fig. 3(b)] time scale for the case $M=100$, $L_x=15$, and $L_y=3$. The initial condition for slow variables is set to be $X(0)=L_x/4$, $P(0)=0$, $H_L(0)=12$, and $H_R(0)=6$. Theoretical results are obtained by solving Eqs. (25)–(27) under the initial condition above. It is naturally conceived that slow variables evolve more slowly as M increases and relaxation in each box is expected to become more rapid as the density in the box increases. From these, we expect that the quasiequilibrium assumption becomes more appropriate in the case where M is large and L_x is small. To see this aspect of the parameter dependence, $X(t)$ for the case $M=10^4$ and $L_x=6$, which is more favorable for satisfaction of the quasiequilibrium assumption than the case of Fig. 3, is shown in Fig. 4 in a short [Fig. 4(a)], a long [Fig. 4(b)], and a very long [Fig. 4(c)] time scale. Compared with Fig. 3, Fig. 4 shows that Eq. (25)–(27) reproduces results of numerical experiments more satisfactorily as was expected.

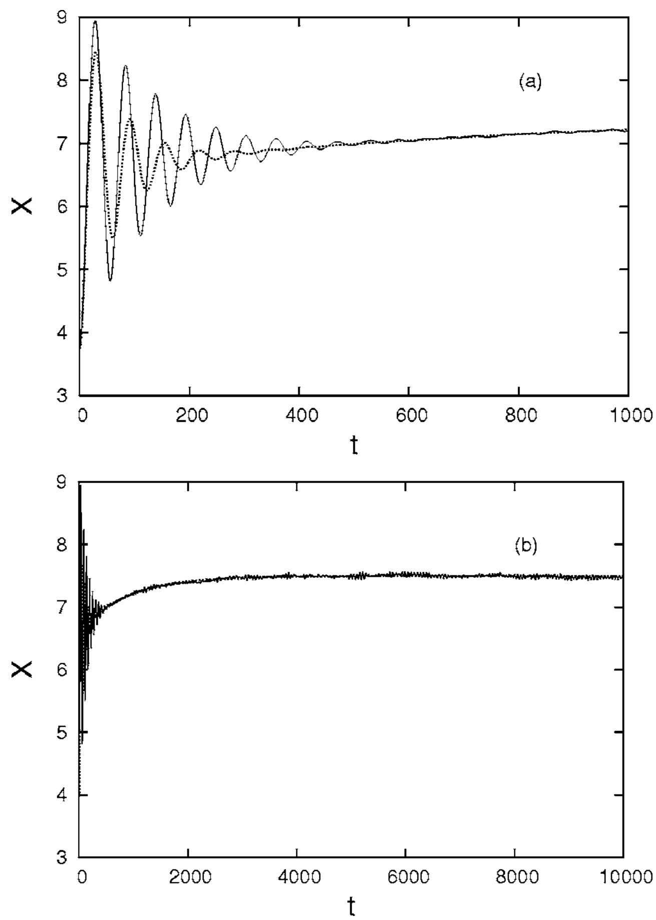

FIG. 3. $X(t)$ from theory (dotted curves) and computer experiments (solid curves) for the case $M=100$, $m=1$, $L_x=15$, and $L_y=3$. The initial condition is chosen to be $X(0)=L_x/4$, $P(0)=0$, $H_L(0)=12$, and $H_R(0)=6$.

In Fig. 5, we show time evolution of H_L and H_R for the system studied in Fig. 4. Although oscillatory behaviors of $H_L(t)$ and $H_R(t)$, shown in the insets, are fairly well reproduced by our theory, we observe that our theory overestimates $H_L(t=\infty)$ and $H_R(t=\infty)$ by 1. This results from the fact that our theory, Eqs. (25)–(27), neglects effects of fluctuations and $P(t=\infty)=0$ instead of $\langle P^2(t=\infty)/(2M)\rangle=2$.

We next consider pressure on the piston. The time evolution of the pressure on the piston due to particles in the left (right) box, denoted by $p_{L(R)}(X,H_{L(R)})$, is shown in Fig. 6. In the theoretical calculation, $p_L(X,H_L)$ is given by Eq. (15). On the other hand, in the simulation, $p_L(X,H_L)$ is obtained as a

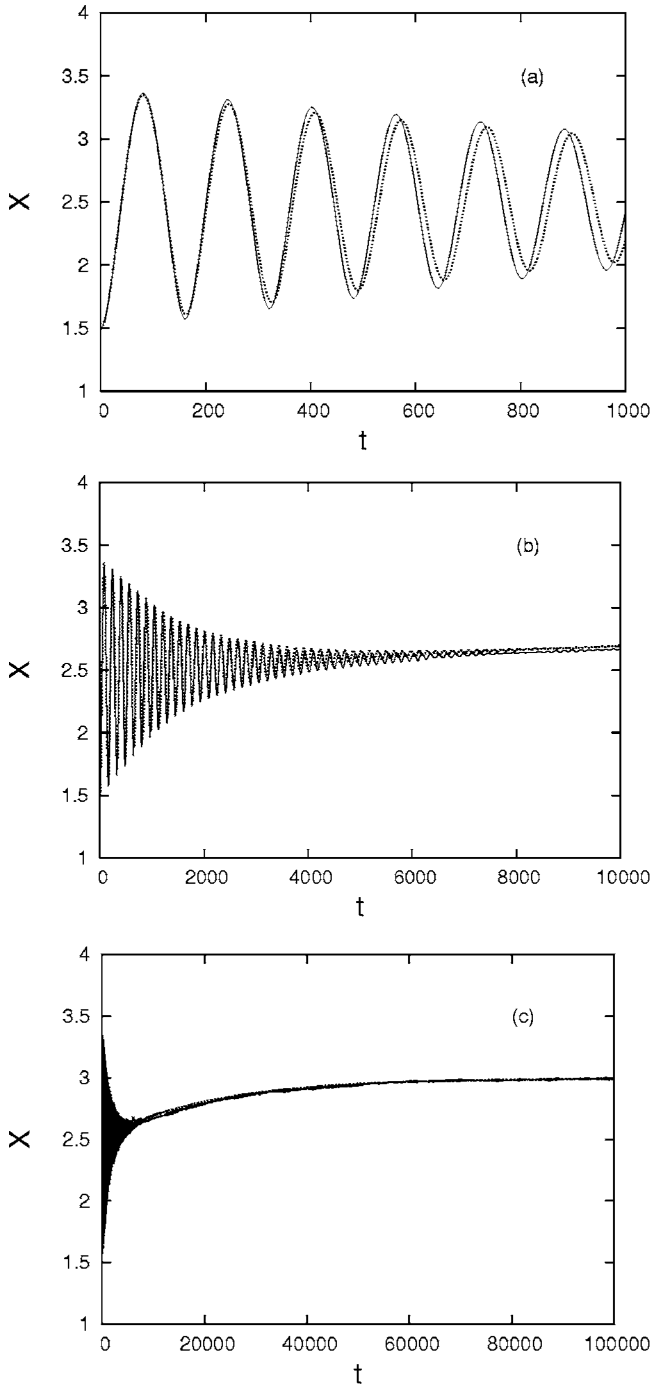

FIG. 4. $X(t)$ from theory (dotted curves) and computer experiments (solid curves) for the case $M=10000$, $m=1$, $L_x=6$, and $L_y=3$. The initial conditions for slow variables are the same as those in Fig. 3.

short-time average of the pressure exerted on the piston by hard disks in the left compartment. $p_R(X,H_R)$ can be obtained similarly. Initially $p_L(X(0),H_L(0))=8.32$ is quite different from $p_R(X(0),H_R(0))=0.68$ and the piston starts moving to the direction of the box with lower pressure and overshoots, resulting in the oscillations (insets). As the system approaches a mechanical equilibrium state the difference in pressure becomes very small and the oscillation becomes

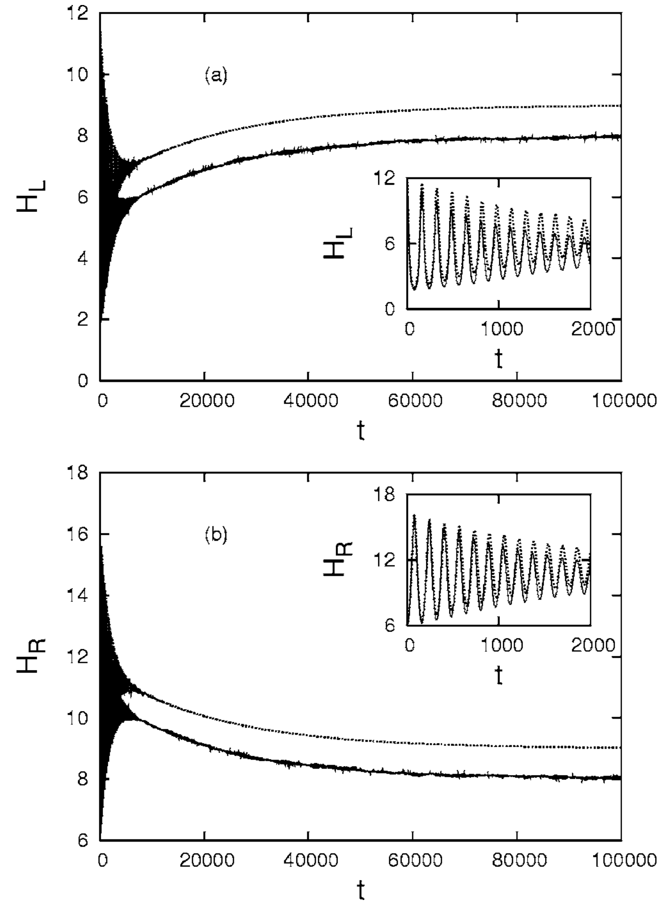

FIG. 5. $H_L(t)$ and $H_R(t)$ from theory (dotted curves) and computer experiments (solid curves) for the system treated in Fig. 4: (a) $H_L(t)$ and (b) $H_R(t)$.

no longer visible. In view of the fact that our theory has no adjustable parameters, we may say that it can reproduce the experimental results well.

Let us discuss the dynamics of the piston semiquantitatively based on the mass-ratio expansion, which has been playing important roles for studies of an adiabatic piston [4–6]. In Eq. (13) we note that the range of integration $\int_L dp_x$ is $\sqrt{2mH_L} \geq p_x > mP/M$. Since P may be considered to be of order $\sqrt{M}$, we put $\epsilon = 1/\sqrt{M}$ and F_L and F_R can be easily expanded in ϵ. Technically one expresses $\int_L dp_x$ as $\int_0^{\sqrt{2mH_L}} - \int_0^{mP/M}$ and the second term is easily Taylor expanded in $mP/M \simeq O(\epsilon)$. Following these procedures we have formally an expansion

$$\frac{dP}{dt} = F_0 + F_1 + F_2 + \cdots , \tag{28}$$

where F_n represents the terms of order ϵ^n.

Let us first consider the piston dynamics to $O(\epsilon^0)$,

$$F_0 = \frac{M}{m+M}\left[\rho_L\left(X - \frac{d}{2}\right)T_L - \rho_R\left(X + \frac{d}{2}\right)T_R\right]$$
$$\equiv \frac{M}{m+M}[p_L(X,H_L) - p_R(X,H_R)]L_y, \tag{29}$$

where $T_{L(R)} \equiv H_{L(R)}/2$ and we use Eq. (14) to obtain the last

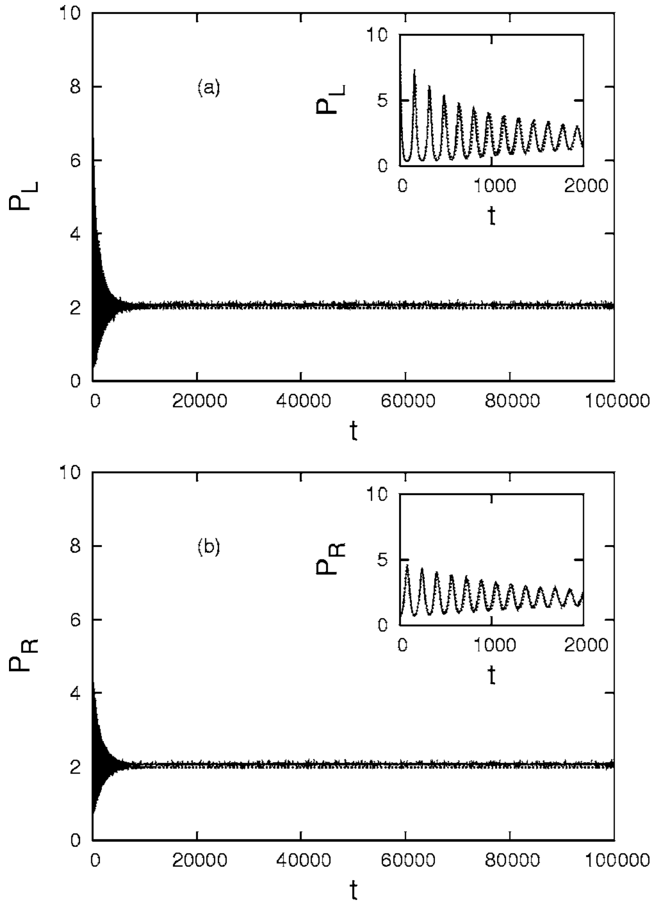

FIG. 6. $p_L(t)$ and $p_R(t)$ from theory (dotted curves) and computer experiments (solid curves) for the system treated in Fig. 4: (a) $p_L(t)$ and (b) $p_R(t)$.

expression. Similarly we expand $W_{L(R)}(a)$ in Eq. (25) to first order in ϵ:

$$\frac{dH_L}{dt} = -\frac{MPL_y p_L(X,H_L)}{(m+M)^2}, \quad \frac{dH_R}{dt} = \frac{MPL_y p_R(X,H_R)}{(m+M)^2}. \tag{30}$$

In Fig. 7 we show $X(t)$ obtained from Eqs. (25) and (28)–(30) in which $m+M$ is approximated by M for the system studied in Fig. 4. $X(t)$ thus obtained oscillates without damping, and its oscillation period is in agreement with one obtained from Eqs. (25)–(27). However, we see that the system can not relax to a mechanical or thermal equilibrium state.

To $O(\epsilon^1)$ we have

$$F_1 = -\zeta P, \ \zeta = \frac{4}{m+M}\left[\rho_L \int_0^{\sqrt{2mH_L}} dp_x p_x f_{eq}(p_x|H_L) + \rho_R \int_0^{\sqrt{2mH_R}} dp_x p_x f_{eq}(p_x|H_R)\right]. \tag{31}$$

Thus we see that it takes time (at least) of order $1/\epsilon^2$ for relaxation to equilibrium and this is much longer than the oscillation period $\tau_{osc} \simeq 1/\epsilon$. Finally to $O(\epsilon^2)$ we have

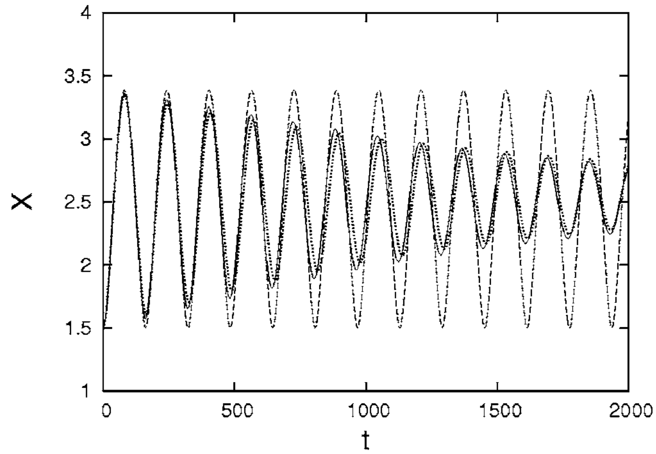

FIG. 7. $X(t)$ obtained from Eqs. (29) and (30) (dashed curve) for the system treated in Fig. 4. Solid and dotted curves are the same as those in Fig. 4.

$$F_2 = (\rho_L - \rho_R)P^2\left(\frac{m}{M^2}\right) = \left(\frac{p_L(X,H_L)}{T_L} - \frac{p_R(X,H_R)}{T_R}\right)L_y P^2\left(\frac{m}{M^2}\right). \tag{32}$$

This shows that the piston moves in the direction of hotter box after mechanical equilibrium is established through $p_L(X,H_L)=p_R(X,H_R)$. This result is well known for an "adiabatic" piston, and simulation results in Figs. 3 and 4 are consistent with Eq. (32).

As a function of the number of hard disks, n_L, and the energy H_L in the left box, the momentum distribution function $f_{eq}(p_x|H_L)$ is generally expressed as [28,29]

$$f_{eq}(p_x|H_L) = \frac{\Gamma(n_L)}{(2m\pi H_L)^{1/2}\Gamma(n_L-1/2)}\left[1 - \frac{p_x^2}{2mH_L}\right]^{n_L-3/2}, \tag{33}$$

where $\Gamma(x)$ is a gamma function. In the limit $n_L \to \infty$ with fixed H_L/n_L, Eq. (33) becomes Maxwellian,

$$f_{eq}(p_x|H_L) = \frac{\exp[(p_x)^2/(2mT_L)]}{(2\pi m T_L)^{1/2}}, \tag{34}$$

with $T_L/2 = H_L/(2n_L)$. This applies also for $f_{eq}(p_x|H_R)$. If we expand F_L+F_R in terms of the smallness parameter $\epsilon \equiv 1/\sqrt{M}$ just as we did above, it is confirmed straightforwardly that the systematic force F_L+F_R on the piston has precisely the expansion obtained before [5] by the method of Van Kampen [30]. Thus we notice that the general expression (13) for the (average) force on the piston gives a concise explanation for directional (to a hotter region) movement of an adiabatic piston.

In this paper we derived the Fokker-Planck equation (24) with the exact partition function Z_2 fully taken into account. We calculated the streaming terms exactly and the diffusion terms approximately neglecting cross correlation functions and effects of correlations among successive collisions in the system. The streaming or systematic terms, which correspond to the Euler equation for hydrodynamics, reproduce experimental results fairly well as shown in Figs. 3–6. The diffusion terms, which were left untouched, deserve careful studies in view of our recent work on an adiabatic piston where molecular dynamics simulations are compared with a Langevin equation [19].

ACKNOWLEDGMENTS

One of the authors (T.M.) expresses his gratitude to G. Hu and H. Li for useful discussions.

APPENDIX: MORI'S THEORY FOR A MICROCANONICAL ENSEMBLE

Let us first consider time evolution of a dynamical variable $\hat{A}(t)$,

$$\frac{d\hat{A}(t)}{dt} = L\hat{A}(t), \quad \hat{A}(t) = \exp(Lt)\hat{A}(0), \tag{A1}$$

where L represents a Liouville operator for a Hamiltonian system with (time-independent) Hamiltonian $\hat{H}$. It is noted that L operates on the initial phase Γ at time $t=0$. Thus $\hat{A}(t)$ is considered to a function of both time t and Γ, which is not explicitly written here. Introducing a projection operator $\mathcal{P}$ by $\mathcal{P}\hat{B}=\langle\hat{B}\hat{A}(0)\rangle\langle\hat{A}(0)\hat{A}(0)\rangle^{-1}\hat{A}(0)$ with $\langle\hat{X}\rangle$ denoting a microcanonical average $\langle\hat{X}\rangle=Z^{-1}\int d\Gamma\hat{X}\delta(\hat{H}-H)$, we have, with $\mathcal{Q}=1-\mathcal{P}$,

$$\frac{d\hat{A}(t)}{dt} = \exp(Lt)[\mathcal{P}L\hat{A}(0) + \mathcal{Q}L\hat{A}(0)]. \tag{A2}$$

The first term on the right-hand side (RHS) of Eq. (A2) is rewritten as

$$\exp(tL)\langle L\hat{A}(0)\hat{A}(0)\rangle\langle\hat{A}(0)\hat{A}(0)\rangle^{-1}\hat{A}(0) = \langle L\hat{A}(0)\hat{A}(0)\rangle\langle\hat{A}(0)\hat{A}(0)\rangle^{-1}\hat{A}(t) \equiv \Omega\hat{A}(t), \tag{A3}$$

where we note that $\exp(tL)C=C\exp(tL)$ when C is a constant.

If we use the fact $L=\mathcal{P}L+\mathcal{Q}L$ and define $L_1\equiv\mathcal{P}L$, $L_2\equiv\mathcal{Q}L$, it is readily checked that

$$\exp(tL) = \exp(tL_2) + \int_0^t ds\, \exp[(t-s)L]L_1\exp(sL_2). \tag{A4}$$

This is used to transform the second term on the RHS of Eq. (A2) to

$$\left(\exp(tL_2) + \int_0^t ds\, \exp[(t-s)L]L_1\exp(sL_2)\right)\mathcal{Q}L\hat{A}(0) = \hat{N}(t) + \int_0^t ds\, \exp[(t-s)L]L_1\hat{N}(s), \tag{A5}$$

where we define $\hat{N}(t)$ by

$$\hat{N}(t) \equiv \exp(tL_2)\hat{N}(0) \tag{A6}$$

with

$$\hat{N}(0) \equiv \mathcal{Q}L\hat{A}(0) = L\hat{A}(0) - \Omega\hat{A}(0). \tag{A7}$$

It is noticed that $L_1\hat{N}(s)$ in Eq. (A5) is readily written as

$$L_1\hat{N}(s) = \langle L\hat{N}(s)\hat{A}(0)\rangle\langle\hat{A}(0)\hat{A}(0)\rangle^{-1}\hat{A}(0). \tag{A8}$$

If one notes that L is expressed in terms of a pair of Poisson brackets with $\hat{H}$ and $L\delta(\hat{H}-H)=0$, we obtain using partial integration that

$$\langle L\hat{N}(s)\hat{A}(0)\rangle = -\langle\hat{N}(s)L\hat{A}(0)\rangle = -\langle\hat{N}(s)\hat{N}(0)\rangle, \tag{A9}$$

where we used the fact that $\hat{N}(s)$ is orthogonal to $\hat{A}(0)$.

From the above we have

$$\frac{d\hat{A}(t)}{dt} = \Omega\hat{A}(t) - \int_0^t ds\,\phi(t-s)\hat{A}(s) + \hat{N}(t), \tag{A10}$$

where the damping function $\phi(t)$ is defined by

$$\phi(t) \equiv \langle\hat{N}(t)\hat{N}(0)\rangle\langle\hat{A}(0)\hat{A}(0)\rangle^{-1}. \tag{A11}$$

If $\hat{A}$ is a (column) vector with N components—i.e., $\hat{A}=(\hat{A}_1,\ldots,\hat{A}_N)^T$—the projection operator $\mathcal{P}$ is introduced by

$$\mathcal{P}\hat{B} = \sum_{i,j}\langle\hat{B}\hat{A}_i(0)\rangle[\langle\hat{A}(0)\hat{A}(0)\rangle^{-1}]_{i,j}\hat{A}_j \tag{A12}$$

and Eq. (A10) for ith component $(i=1,\ldots,N)$ of $\hat{A}$ is written as

$$\frac{d\hat{A}_i(t)}{dt} = \sum_j\Omega_{i,j}\hat{A}_j(t) - \sum_j\int_0^t ds\,\phi_{i,j}(t-s)\hat{A}_j(s) + \hat{N}_i(t), \tag{A13}$$

with Ω and $\phi(t)$ being an $N\times N$ matrix—e.g., $\Omega_{i,j}=\Sigma_k\langle L\hat{A}_i\hat{A}_k\rangle[\langle\hat{A}(0)\hat{A}(0)\rangle^{-1}]_{k,j}$. Finally, if $\hat{A}$ is labeled not by a discrete index i but by a continuous parameter like $A_a=\delta(\hat{A}-a)$ with $-\infty<a<\infty$, we may simply replace Σ_i by $\int da$ in Eq. (A13).

[1] H. B. Callen, *Thermodynamics* (Wiley, New York, 1963).
[2] E. H. Lieb, Physica A **263**, 491 (1999).
[3] J. Piasecki and C. Gruber, Physica A **265**, 463 (1999).
[4] C. Gruber and J. Piasecki, Physica A **268**, 412 (1999).
[5] T. Munakata and H. Ogawa, Phys. Rev. E **64**, 036119 (2001).
[6] P. Meurs, C. Van den Broeck, and A. Garcia, Phys. Rev. E **70**, 051109 (2004).
[7] M. M. Mansour, C. Van den Broeck, and E. Kestemont, Europhys. Lett. **69**, 510 (2005).
[8] M. M. Mansour, A. L. Garcia, and F. Baras, Phys. Rev. E **73**, 016121 (2006).
[9] E. Kestemont, C. Van den Broeck, and M. M. Mansour, Europhys. Lett. **49**, 143 (2000).
[10] C. Gruber, S. Pache, and A. Lesne, J. Stat. Phys. **108**, 669 (2002).
[11] C. Gruber, S. Pache, and A. Lesne, J. Stat. Phys. **112**, 1177 (2003).
[12] J. A. White, F. L. Román, A. González, and S. Velasco, Europhys. Lett. **59**, 479 (2002).
[13] Y. G. Sinai, Theor. Math. Phys. **121**, 1351 (1999).
[14] A. I. Neishtadt and Y. G. Sinai, J. Stat. Phys. **116**, 815 (2004).
[15] Y. G. Sinai, *Dynamical Systems II: Ergodic Theory with Applications to Dynamical Systems and Statistical Mechanics* (Springer-Verlag, Berlin, 1989).
[16] L. D. Gelb, K. E. Gubbins, R. Radhakrishnan, and M. Sliwinska-Bartkowiak, Rep. Prog. Phys. **62**, 1573 (1999).
[17] There are some molecular dynamics simulation studies on dynamical properties of a few-body systems and these works are closely related to our work in this paper. Since all the dynamical correlations present among particles are included, we may regard the results of these computer experiments as exact [A. Awazu, Phys. Rev. E **63**, 032102 (2001); S.-H. Suh and S.-C. Kim, *ibid.* **69**, 026111 (2004)].
[18] R. K. Bowles, K. K. Mon, and J. Percus, J. Chem. Phys. **121**, 10668 (2004).
[19] H. Li, D. He, Z. Cao, Y. Zhang, T. Munakata, and G. Hu, Phys. Rev. E **71**, 061103 (2005).
[20] T. Munakata and G. Hu, Phys. Rev. E **65**, 066104 (2002).
[21] Z. Cao, H. Li, T. Munakata, D. He, and G. Hu, Physica A **334**, 187 (2004).
[22] H.-H. Li, Z.-J. Cao, D.-H. He, and G. Hu, Europhys. Lett. **67**, 335 (2004).
[23] H. Mori, Prog. Theor. Phys. **33**, 423 (1965).
[24] H. Mori and H. Fujisaka, Prog. Theor. Phys. **49**, 764 (1973).
[25] I. Z. Fisher, *Statistical Theory for Liquids* (Chicago University Press, Chicago, 1964).
[26] H. Risken, *The Fokker-Planck Equation: Methods of Solution and Applications* (Springer, Berlin, 1996).
[27] H. Grad, Commun. Pure Appl. Math. **2**, 331 (1949).
[28] J. R. Ray and H. W. Graben, Phys. Rev. A **44**, 6905 (1991).
[29] F. L. Román, J. A. White, and S. Velasco, Phys. Rev. E **51**, 6271 (1995).
[30] N. G. Van Kampen, Can. J. Phys. **39**, 551 (1961).