# Chaos and irreversibility in a conservative nonlinear dynamical system with a few degrees of freedom

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The motion of an elastic pendulum with two degrees of freedom has been investigated in the vicinity of a separatrix, using the Liouville equation. Even for this simple system, an irreversible kinetic equation of the Fokker-Plank type for the momentum-distribution function has been obtained in the limit of a stiff pendulum. This equation describes a monotonic approach to the "microcanonical equilibrium state" for a given energy surface. The diffusion coefficient for the energy of the unperturbed pendulum in this work is directly related to that obtained by Chirikov's heuristic argument.

## I. INTRODUCTION

The purpose of this paper is to derive an irreversible kinetic equation which describes the long-time behavior of a conservative nonlinear dynamical system with a few degrees of freedom near a separatrix. Since Boltzmann[1] showed the $H$ theorem in his kinetic equation for a dilute gas system with a large number of degrees of freedom, compatibility of the second law of thermodynamics with the basic laws of dynamics has been the object of controversy.[2] It is well understood, at present, that Boltzmann's derivation of the kinetic equation was basically phenomenological. The main step involved is the replacement of the dynamical laws by a physically plausible stochastic mechanism: the "Stosszahlansatz."

An important development after Boltzmann's derivation has been achieved by Van Hove[3] in quantum systems and by Prigogine and his colleagues[4–7] in classical systems. Collecting the most divergent terms in the limit of time $t \rightarrow \infty$ in a perturbation series, they have derived irreversible kinetic equations. An essential development and distinction of their derivation from others[8–12] is that they have clearly distinguished roles of dynamics in evolution of the system from roles of statistics. The statistical assumption involved in their theory was imposed only on the initial conditions. With this distinction, Prigogine[5] has summarized a dynamical condition for the irreversibility as the "dissipativity condition," that is the "condition of the existence of nonvanishing *collision operator*." He has also emphasized the importance of analytical restrictions on the initial conditions of the system to have the irreversibility.

However, the arguments by Van Hove and by Prigogine and his colleagues have been concerned with systems having an infinite number of degrees of freedom because of the following reasons. First, complexity of the motion quickly increases, as the number of degrees of freedom increases. It is natural to suppose that the irreversibility is a result of the complexity. Second, one of the necessary conditions to obtain the nonvanishing collision operators is that the Liouville operator of the system should have a continuous spectrum. This condition is satisfied if we consider a system in the thermodynamic limit, i.e., a system enclosed in an infinitely large box with a finite density.

Independently of the development in the nonequilibrium statistical mechanics, recent study of dynamical systems with a finite number of degrees of freedom reveals the complexity of the motion in nonlinear systems, even when they have only two degrees of freedom. When the well-known difficulty of the resonance effect in the perturbation theory for nonintegrable systems (that is, the difficulty of the small denominator) was overcome by Kolmogorov,[13] by Arnol'd,[14] and by Moser[15] (i.e., the KAM theory), the following was found: In every $\epsilon$-neighborhood of a given point in phase space through which passes a trajectory of a certain type, one might find trajectories corresponding to asymptotically different behavior no matter how small $\epsilon$ is. For a given Hamiltonian, there are various types of motion possible, each with a nonvanishing measure. This complexity is strikingly illustrated by computer simulations of Hénon and Helies,[16] Ford, and others.[17]

It seems to us from these findings that an "embryo" of the irreversibility exists already in such complex motion in nonlinear conservative systems with two degrees of freedom. Our purpose is, thus, to show this embryo and add a new mechanism of the irreversibility, i.e., the nonlinearity, by extending Prigogine's perturbation theory into the form that makes it possible to treat finite nonlinear systems whose periodicity depends on energy.

One of the conspicuous distinctions of Prigogine's perturbation theory from other theories (e.g., the KAM theory) is that this theory deals with the evolution of the Gibbs ensemble. The classical approach to dynamical systems is to study individual trajectories. However, when the motion starts from an unstable region of phase space, different initial conditions, which lie arbitrarily close to each other in phase space, may yield exponentially diverging trajectories.[18] In this situation the concept of deterministic motion along trajectories ceases to be a physically meaningful idealization.[19] This makes it necessary to go to a probabilistic description of physical states in terms of the Gibbs ensemble.

Another conspicuous distinction is that this theory chooses time as one of the expansion parameters in the perturbation series, and collects the most divergent terms coming from the resonance effect in the limit as the time goes to infinity. This makes it possible to deal with the evolution of the system in the resonance region in phase space, where the KAM theory does not work. By using a simple example, we show that the irreversibility is a result of the resonance effect, when the resonance value of the momenta in phase space is densely distributed.

As an example to illustrate our extension of Prigogine's perturbation theory, we consider an autonomous system: an elastic pendulum with two degrees of freedom with a linear spring which obeys Hooke's law, as shown in Fig. 1. Here, $\theta$ denotes angular displacement of the pendulum from its stable equilibrium position at bottom, $x$ is the displacement of the spring from its natural length $l$, and $m$ is the mass. For sufficiently stiff spring with large natural frequency, we show that the Hamiltonian of the system simply consists of three terms: the Hamiltonian of the unperturbed pendulum (i.e., the pendulum with the fixed length $l$), the Hamiltonian of the linear spring, and a small interaction between the unperturbed pendulum and the spring. Then we focus our attention to the vicinity of the separatrix of the unperturbed pendulum in phase space (i.e., a trajectory that separates rotational motion of the pendulum from librational motion). In time evolution the pendulum stays almost all the time around the top ($\theta \simeq \pi$) without interaction, and passes quickly the bottom ($\theta = 0$), where the centrifugal force becomes maximum, with a short interaction time.

The existence of the separatrix is a typical property of nonliner systems. A complex deformation of the unperturbed separatrix by a small perturbation has been already noticed about 100 years ago by Poincaré.[20] Indeed, we show that there exists an unstable region, called the "stochastic layer," around the separatrix. The unstable motion is confined in the stochastic layer. Then, if the initial condition of the ensemble is chosen in a small region inside this unstable region, as it evolves in time, the ensemble stretches in a direction parallel to the unperturbed separatrix and expands in the vertical direction, as shown in Fig. 2. For the case of sufficiently small interaction, the stretch in the parallel direction is rather systematic, and is mainly a result of nonlinearity in the unpertubed system where the periodicity of the system depends on the energy, so that this process exists even when the interaction does not exist. On the other hand, the expansion in the vertical direction exists only when the interaction exists. This is the process in which we are mainly interested in this paper. We show that this process is described by an irreversible kinetic equation which reduces to a Fokker-Planck equation for sufficiently small interaction; the diffusion coefficient of the unperturbed energy of the pendulum characterizing this irreversible process is given by

$$D_{H_1} = \frac{72\pi^2 H_2}{\mu^2 \sqrt{H_1}\, T(H_1)} e^{-\pi/\mu\sqrt{H_1}} \tag{1.1}$$

with the condition

$$\mu = \frac{\omega_0}{\Omega} \ll 1 \ . \tag{1.2}$$

Here, $\Omega$ is the natural frequency of the linear spring, $\omega_0 = \sqrt{g/l}$ is the natural frequency of the harmonic pendulum for small amplitude, and $T(H_1) = [\ln(16/|H_1 - 1|)]^{-1}$ is the period of the rotation, or the half-period of the libration of the unperturbed pendulum near the separatrix. The variables $H_1$ and $H_2$ are dimensionless energies of the unperturbed pendulum and the spring measured with a unit of the energy of the unperturbed pendulum at the separatrix. If we replace $T(H_1)$ in Eq. (1.1) by its average value in the stochastic layer, we show that the diffusion coefficient $D_{H_1}$ coincides with the one obtained by Chirikov's heuristic argument[18] with the assumption of ergodicity. We further show that our Fokker-Planck equation describes a monotonic approach to the microcanonical equilibrium state for a given energy surface.

The program of technical argument in this paper is the following. In Sec. II we introduce a well-defined frame-

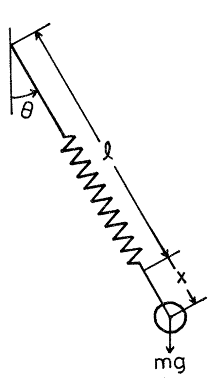


FIG. 1. Elastic pendulum.

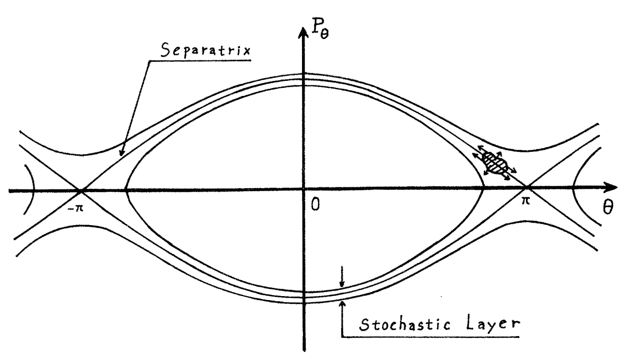


FIG. 2. Diffusion process in phase space: This is a cross section in phase space. Diffusion process in the vertical direction to the unperturbed separatrix is a result of the resonant interaction. Stretch process in the parallel direction is rather systematic, and is mainly a result of nonlinearity in the unperturbed system.

work (i.e., canonical variables) to describe the motion of the elastic pendulum in the vicinity of the separatrix. A difficulty encountered in treating the motion around the separatrix is that the action-angle variables of the unperturbed pendulum diverge at the separatrix. We show that there is a set of canonical variables—instead of the action-angle variables—that is well defined and continuous at the separatrix and make the Hamiltonian of the unperturbed pendulum cyclic. In these variables, however, the interaction term is yet nonanalytic at the separatrix; higher-order derivatives of this term in the new momentum diverge, due to the logarithmic divergence of the period of the unperturbed pendulum at the separatrix.

At the same time, however, we show that the interaction term as a function of the parameter $\mu$ in Eq. (1.2) has an essential singularity at $\mu=0$. This singularity appears as an infinitely rapid oscillating factor in the interaction term. Because of this rapid oscillation, the effect of the interaction damps very quickly to zero as the value of $\mu$ decreases. We emphasize the importance of this essential singularity to overcome the above-mentioned logarithmic singularity in the perturbation series at the separatrix.

Using the new canonical variables we show that the value of the energy at the separatrix of the unperturbed pendulum is an accumulation point of infinitely many resonance values of the energy around the separatrix. We further show that these resonances give rise to an infinite number of singular motions (i.e., stable and unstable of periodic motions). The distribution of these singular motions is studied by constructing a Poincaré map, called the "whisker map," similar to the one obtained by Chirikov.[18] From this map we estimate the width of the stochastic layer in phase space.

In Sec. III we extend Prigogine's perturbation theory such that we may treat a nonlinear system, periodicity of which depends on the momentum. Using the new canonical variables, we show that the discreteness of the spectrum of the unperturbed Liouville operator tends to zero with decreasing difference of the energy of the unperturbed pendulum from the separatrix, so that we may construct a nonvanishing collision operator to obtain an irreversible kinetic equation for the momentum distribution function in the stochastic layer. In the limit of small interaction, we show that the contribution of the interaction comes only when the resonance condition between the unperturbed frequencies of the pendulum and the spring is satisfied.

In Sec. IV we investigate some properties of our kinetic equation. In a certain choice of the variables, we show that the kinetic equation reduces to the one-dimensional Fokker-Planck equation for the distribution function of the energy of the unperturbed pendulum. Finally, we compare the diffusion coefficient Eq. (1.1) with the one obtained by Chirikov's heuristic argument.[18] Then we show the two coefficients are equivalent if we replace the period of the unperturbed pendulum in the diffusion coefficients by its average value in the stochastic layer, and if we assume the microcanonical distribution for the phase of the spring in Chirikov's argument.

In Sec. V we summarize our results and make a few comments on an analogy of characteristic time scales in the elastic pendulum to the ones in a dilute gas system with a short-range interaction.

## II. ELASTIC PENDULUM

We consider the motion of an elastic pendulum with two degrees of freedom, made from a stiff linear spring which obeys Hooke's law, as shown in Fig. 1. The Hamiltonian of the system is given by

$$\tilde{H}=\frac{P_\theta^2}{2ml^2}\frac{1}{(1+x/l)}+ml^2\omega_0^2(1-\cos\theta)-\frac{x}{l}ml^2\omega_0^2\cos\theta+\frac{p_x^2}{2m}+\frac{m\Omega^2x^2}{2}\,, \tag{2.1}$$

where $P_\theta$ and $p_x$ are momenta which are conjugate with $\theta$ and $x$, respectively. We denote time which is conjugate with $\tilde{H}$ by $\tilde{t}$.

Let us measure the energy of the elastic pendulum by the unit of $H_{sx}=2ml^2\omega_0^2$ which is the value of the energy of the unperturbed pendulum at the separatrix. Let $H=\tilde{H}/\tilde{H}_{sx}$, $Y_1=P_\theta/(2ml^2\omega_0)$, $\theta_1=\theta$, $y_2=\Omega J/\tilde{H}_{sx}$, and $\alpha_2=\mu\phi$, where the action-angle variables $(J,\phi)$ of the spring are defined by $x=\sqrt{2J/m\Omega}\cos\phi$ and $p_x=\sqrt{2m\Omega J}\sin\phi$, and $\mu$ is defined in Eq. (1.2). Then, the Hamiltonian, Eq. (2.1), is given in a dimensionless form by

$$H=\frac{Y_1^2}{[1+2\mu\sqrt{y_2}\cos(\alpha_2/\mu)]^2}+\tfrac{1}{2}(1-\cos\theta_1)+y_2-\mu\sqrt{y_2}\cos\theta_1\cos\frac{\alpha_2}{\mu}\,. \tag{2.2}$$

Note that if we regard the dimensionless quantities $H$ and $t=\omega_0\tilde{t}$ as the new Hamiltonian and time, respectively, then the dimensionless variables $Y_1$ and $\theta_1$, and $y_2$ and $\alpha_2$ are canonically conjugate variables to each other, respectively.

On a given energy surface $H=E$, the energy of the spring, $y_2$, has the maximum value at $Y_1=\theta_1=\alpha_2=0$ such that

$$(y_2)_{\max}=\tfrac{1}{4}[\mu+(\mu^2+4E)^{1/2}]^2\,. \tag{2.3}$$

Let us assume the inequality in Eq. (1.2) and $O(E)=1$. Then, we approximate the Hamiltonian, Eq. (2.2), to first order of $x/l=2\mu\sqrt{y_2}\cos(\alpha_2/\mu)$ and obtain

$$H=H_0+\lambda V\,, \tag{2.4}$$

where $H_0=H_1+H_2$ with

$$H_1=Y_1^2+\tfrac{1}{2}(1-\cos\theta_1)\,, \tag{2.5a}$$

$$H_2=y_2\,, \tag{2.5b}$$

and the interaction $\lambda V$ is given by

$$\lambda V=-\lambda\mu(4Y_1^2+\cos\theta_1)\sqrt{y_2}\cos\frac{\alpha_2}{\mu}\,, \tag{2.6}$$

where we have introduced the parameter $\lambda$ to indicate the order of the interaction. The elastic pendulum corresponds to the case of $\lambda=1$ in Eq. (2.4).

$H_1$ in Eq. (2.5a) is the Hamiltonian of the unperturbed pendulum. In this representation the energy of the unperturbed pendulum on the separatrix is normalized such that $H_1=1$. The region of interest in phase space of the elastic pendulum is specified by the inequality $|H_1-1| \ll 1$.

We now introduce new canonical variables $(y_1,\alpha_1)$ in which the Hamiltonian of the unperturbed pendulum becomes cyclic. The variables are defined through the following canonical transformations:

(i) for the rotation $(0 \le c < 1)$

$$\sin\frac{\theta_1}{2}=\pm\mathrm{sn}\left[\frac{\alpha_1}{2},c\right], \quad Y_1=\pm y_1\mathrm{dn}\left[\frac{\alpha_1}{2},c\right]; \tag{2.7a}$$

(ii) for the separatrix $(c=1)$

$$\sin\frac{\theta_1}{2}=\pm\tanh\frac{\alpha_1}{2}, \quad Y_1=\pm y_1\mathrm{sech}\frac{\alpha_1}{2}; \tag{2.7b}$$

(iii) for the libration $(c>1)$

$$\sin\frac{\theta_1}{2}=\frac{1}{2\sqrt{c}}\mathrm{sn}\left[\frac{\sqrt{c}}{2}\alpha_1,\frac{1}{c}\right], \quad Y_1=y_1\mathrm{cn}\left[\frac{\sqrt{c}}{2}\alpha_1,\frac{1}{c}\right], \tag{2.7c}$$

where $c$ is related to $y_1$ by

$$c=\frac{1}{y_1^2} \tag{2.8}$$

and the new Hamiltonian of the unperturbed pendulum is

$$H_1=y_1^2 \tag{2.9}$$

for any value of $c$. Here $\mathrm{sn}(u,c)$, $\mathrm{cn}(u,c)$, and $\mathrm{dn}(u,c)$ are the Jacobi elliptic functions and $c$ in Eq. (2.7a) and $c^{-1}$ in Eq. (2.7c) are square of the modulus of the elliptic function.[21] Each sign in Eqs. (2.7a) and (2.7b) corresponds to each direction of the motion in the rotation and on the separatrix: We assume $y_1 \ge 0$ in this paper, so that the + sign corresponds to counterclockwise motion.

Note that our canonical transformations, Eq. (2.7), are well defined and continuous at $H_1=1$. This property is not satisfied by the ordinary action-angle variables of the unperturbed pendulum that diverge at the separatrix. The relation between our variables and the ordinary action-angle variables is discussed in the Appendix.

The period of the rotation $T_R$ and the half-period of the libration $T_{L/2}$ of the unperturbed pendulum are given by

$$T_R=2\sqrt{c}K(c), \quad T_{L/2}=2K(c^{-1}), \tag{2.10}$$

respectively, where $K$ is the complete elliptic integral of the first kind. Near the separatrix, i.e., $c \simeq 1$, $T_R$ and $T_{L/2}$ are both approximated by

$$T_{c'}=\ln\left[\frac{16}{|c'|}\right], \tag{2.11}$$

where

$$c'=1-c \tag{2.12}$$

is the square of the complementary modulus of the elliptic function for $0 \le c \le 1$. For $c>1$ and $|c'| \ll 1$, the square of the complementary modulus of $c^{-1}$ is approximated by $|c'|$. The rotational motion corresponds to the case of $c'>0$. For sufficiently small $|c'|$ we have $c' \simeq H_1-1$, i.e., $c'$ is just the difference of the energy of the unperturbed pendulum from the separatrix.

Applying the canonical transformation in Eq. (2.7) to the Hamiltonian of the elastic pendulum in Eq. (2.4) we obtain the new Hamiltonian

$$H=y_1^2+y_2+\lambda\mu y_1^2[2-c-6f(\alpha_1,c)]\sqrt{y_2}\cos\frac{\alpha_2}{\mu}, \tag{2.13}$$

where

$$f(\alpha_1,c)=\begin{cases}\mathrm{dn}^2\left[\dfrac{\alpha_1}{2},c\right], & c' \ge 0\\[2ex] \mathrm{cn}^2\left[\dfrac{\sqrt{c}}{2}\alpha_1,\dfrac{1}{c}\right], & c'<0.\end{cases} \tag{2.14}$$

Because the system is periodic with respect to $\alpha_1$ we may restrict the region of $\alpha_1$ to $|\alpha_1| \le T(c)/2$ for given $c$ in the phase space without any loss of generality, where $T(c)$ is the period of the function $f(\alpha_1,c)$ and is given by $T(c)=4K(c)$ for $c' \ge 0$ and $T(c)=4c^{-1/2}K(c^{-1})$ for $c'<0$.

To investigate the long-time evolution of the system around the separatrix, we will apply a perturbation theory to the Hamiltonian, Eq. (2.13). In this paper, however, we will not attempt to justify the applicability of the perturbation theory, but content ourselves with a few remarks on analytic properties of the interaction term in the Hamiltonian, Eq. (2.13). A detailed argument of higher-order approximation of our perturbation theory will be given separately in a forthcoming paper.

We first notice that the interaction has an essential singularity at $\mu=0$, as a function of this parameter. The effect of this singularity appears as an infinitely rapid oscillating factor in the interaction. Because of this rapid oscillation, the effect of the interaction damps very quickly in the limit of $\mu \to 0$.

Second, the interaction has a singularity of the momentum $y_1$ at $y_1=1$ (i.e., at the separatrix, $c=1$) which comes from the logarithmic singularity of the elliptic integrals of the first kind $K$, and the second kind $E$, at this point.[21] Because of this singularity the $m$th-order derivative of the function $f(\alpha_1,c)$ by $c$ diverges in the limit of $c \to 1$ for $m \ge 2$. However, since the zeroth and first derivatives by $c$ are finite in this limit, we may show that the effect of the interaction vanishes at this singular point in the limit of $\mu \to 0$ due to the rapid oscillating factor in the interaction.[22] This implies that we may regard the interaction as a weak perturbation even though we have the singularity at $c=1$.

Finally, the interaction has a singularity of the momentum $y_2$ at $y_2=0$ and at infinity. In order to avoid diverging contribution of the interaction at these points, we assumed that the initial value of $y_2$ is chosen such that $\mu \ll \sqrt{y_2} \ll \mu^{-1}$. We will see later that this condition is always satisfied around the separatrix for sufficiently small $\mu$.

We now study a structure of the phase space around the separatrix. Because $f(\alpha_1,c)$ in the interaction is a periodic function of $\alpha_1$, we can expand it in a Fourier series such that for the $\mathrm{dn}^2$ function

$$\mathrm{dn}^2\left[\frac{\alpha_1}{2},c\right]=\frac{E}{K}+\Delta k\sum_{n=-\infty}^{+\infty}{}' \frac{2n\,\Delta k}{\sinh(2n\,\Delta k\,K')}e^{in\,\Delta k\,\alpha_1} \tag{2.15}$$

and for the $\mathrm{cn}^2$ function

$$\mathrm{cn}^2\left[\frac{\sqrt{c}}{2}\alpha_1,c^{-1}\right]=c\,\mathrm{dn}^2\left[\frac{\sqrt{c}}{2}\alpha_1,c^{-1}\right]+c' \tag{2.16}$$

with the expansion Eq. (2.15), where

$$\Delta k=\frac{\pi}{2K(c)} \tag{2.17}$$

and the prime on the summation sign stands for $n\neq 0$. Therefore, we have an infinite number of resonance interactions between the spring and the unperturbed pendulum. The resonance values of $c'$ are given as solutions of the resonance equation $n\,\Delta k(\partial H_1/\partial y_1)+(1/\mu)(\partial H_2/\partial y_2)=0$. When sufficiently close to the separatrix, i.e., $|c'|\ll 1$, we can solve the resonance equation explicitly, and the resonance values are given by

$$|c'|\simeq 16e^{-2\pi\mu n}\,, \tag{2.18}$$

where $n$ is any integer. This result shows that the separatrix $c'=0$ is an accumulation point of the resonance values of $c'$.

We now show that the resonance interactions give rise to an infinite number of singular motions (i.e., stable and unstable periodic motions) around the separatrix. To find the singular solutions, we first construct a discrete map of the Poincaré surface of section for the variables $y_1$ and $\alpha_2$ on a surface given by $\alpha_1=\alpha_0$ in phase space. The periodic solutions are found as fixed points of the Poincaré map. We here assume that the surface is chosen such that $|\alpha_0|\gg 1$ because of the following reasons. First, we are interested in a phenomena which occurs in longer time scale than a duration of interaction between two degrees of freedom. Second, the time scale that the pendulum spends in the region of $|\alpha_1|\lesssim 1$ (which will be interpreted as the duration of interaction, later) is negligibly small as compared with the time scale of the uncoupled motion in the region of $|\alpha_1|\gg 1$ for sufficiently small $\mu$.

To construct the map, we choose the origin of the time $t=0$ such that $\alpha_1(0)=0$ [i.e., $\theta_1(0)=0$], and assume that the trajectory passes the surface of section at $t=-t_0$ and next at $t=-t_0+T$, i.e., $\alpha_1(-t_0)=\alpha_1(-t_0+T)=\alpha_0$. The increment $\Delta y_1$ of $y_1$ in an interval of the map is given by

$$\Delta y_1=-\int_{-t_0}^{-t_0+T}dt\frac{\partial H}{\partial \alpha_1}\,. \tag{2.19}$$

To evaluate the right-hand side of Eq. (2.19), we approximate the evolution of $\alpha_1(t)$, $y_1(t)$, $\alpha_2(t)$, and $y_2(t)$ by the unperturbed solutions. Then we approximate such that $c=1$, since we are interested in the energy $H_1$ very close to the separatrix. The integrand in Eq. (2.19) is now proportional to the factor $\mathrm{sech}^2 t\tanh t$, which damps exponentially to zero for large $|t|$, and changes most rapidly around the origin, $t=0$. Furthermore, the integrand includes a rapidly oscillating factor $\cos\mu^{-1}(t+t_0+\alpha_2')$, where $\alpha_2'=\alpha_2(-t_0)$ is the initial phase of the spring at the surface of section. This implies that the contribution of the interaction in Eq. (2.19) comes from only a small interval of $t$ around $t=0$. Further, we approximate $T$ by the unperturbed period $T_{c'}$, in Eq. (2.11). Therefore, because of the way we choose the surface of section and the origin of time, the values $t_0$ and $-t_0+T$ are much greater than one. Consequently we may replace the limits of the integration, $-t_0$ and $-t_0+T$, by negative and positive infinity, respectively.

We may interpret this fact that the two degrees of freedom collide in a short interaction time around $t=0$ where the centrifugal force becomes maximum, and move without interaction almost all of the time before and after the collision. We may estimate the duration of the interaction, $t_i$, which may be defined to be the time for which the absolute value of the integrand in Eq. (2.19) decreases to $e^{-1}$ of its maximum value. Neglecting the oscillating factor in the integrand, we obtain $t_i\simeq 1$. This verifies the above replacement of the limits of the integration in Eq. (2.19). This estimate of $t_i$ is also supported by evaluating the singularity of the collision operator, defined in Eq. (3.48a), with respect to $z$.[7] We will estimate it in this point of view after we obtain the explicit form of the collision operator of the elastic pendulum.

Substituting the Fourier integral of $\mathrm{sech}^2 t\tanh t$ in Eq. (2.19) and integrating by $t$ with the above approximation, we ultimately obtain the following result for $\mu\ll 1$:

$$\begin{aligned}\Delta y_1&\simeq -6\lambda\mu\sqrt{y_{20}}\int_{-\infty}^{+\infty}dt\,\mathrm{sech}^2 t\tanh t\times\cos\left[\frac{1}{\mu}(t+t_0+\alpha_2')\right]\\&\simeq 6\pi\lambda\sqrt{y_{20}}\frac{e^{-\pi/2\mu}}{\mu}\sin\left[\frac{1}{\mu}(\alpha_2'+t)\right]\,,\end{aligned} \tag{2.20}$$

where $y_{20}=y_2(-t_0)$.

In approximating the integrand in Eq. (2.20) by the unperturbed solution, we have assumed that the inequality $\mu/\sqrt{y_2(t)}\ll 1$ is always satisfied. We can verify this assumption by estimating the increment $\Delta y_2(t)=y_2(t)-y_{20}$ for $-t_0\le t\le -t_0+T$ in a way similar to the above such that

$$\left|\frac{\Delta y_2(t)}{y_{20}}\right|\simeq\frac{\lambda}{\sqrt{y_{20}}}\left|\int_{-t_0}^{t}dt'(1-6\,\mathrm{sech}^2 t')\sin\left[\frac{1}{\mu}(t'+t_0+\alpha_2')\right]\right|\lesssim 8\lambda\frac{\mu}{\sqrt{y_{20}}}\,, \tag{2.21}$$

where we have replaced $-t_0$ by $-\infty$ in evaluating the second term and neglecting exponentially small contribution for sufficiently small $\mu$. Equation (2.21) is the desired result, because we have assumed the initial condition such that $\mu/\sqrt{y_{20}} \ll 1$. This result shows also that a variation of $y_2$ in an interval of the map is a higher-order effect of the perturbation. Therefore, we neglect this variation in each mapping of $y_1$ and $\alpha_2$ in the lowest-order approximation.

The increment of the phase of the spring $\Delta\alpha_2$ in an interval of the map is approximately estimated by the unperturbed solution of $\alpha_2(t)$ and by $T \simeq T_{c'}$. Then we obtain

$$\Delta\alpha_2 \simeq \ln\frac{8}{|y_1-1|} . \tag{2.22}$$

Now, we can combine the above results to obtain the Poincaré map. Introducing new variables $x=y_1-1$ and $\alpha=\alpha_2'+t_0$, and denoting the variables after an interval of the map by $\bar{x}$ and $\bar{\alpha}$, we arrive at a set of difference equations,

$$\begin{aligned} \bar{x} &= x + w\sin\frac{\alpha}{\mu} , \\ \bar{\alpha} &= \alpha + \ln\frac{8}{|\bar{x}|} \quad (\text{mod } 2\pi\mu) , \end{aligned} \tag{2.23}$$

where

$$w = 6\pi\lambda\sqrt{y_{20}}\frac{e^{-\pi/2\mu}}{\mu} . \tag{2.24}$$

In the second equation in Eq. (2.23) we have substituted $\bar{x}$, for $x$ in order to make the map canonical. Because of the relation $c' \simeq 2x$ for small $c'$, we may also interpret the map, Eq. (2.23), as a map for the pendulum energy $c'$.

Note that a change of sign of $x$ in Eq. (2.23) is equivalent to the shift of $\alpha$ to $\alpha+\mu\pi$ without change of $x$. This implies that the structure of the phase space corresponding to the oscillatory motion is the same as the one for rotational motion, except for the shift of the phase $\alpha$ by $\pi\mu$. Thus, it is sufficient to investigate the case of the rotational motion, $c'>0$, to obtain the whole information of the structure of the phase space around the separatrix. The following statements about the structure of the phase space are, therefore, only for the rotational case.

The fixed solution of the map is now easily obtained by setting $\sin(\alpha/\mu)=0$ and $\ln(8/x)=2\pi\mu n$, where $n$ is any integer. Then, we obtain

$$\alpha = 0 \text{ or } \pi\mu , \quad x = 8e^{-2\pi\mu n} . \tag{2.25}$$

Noting $c' \simeq 2x$, we see that the fixed value of $c'$ is just the resonance value in Eq. (2.18). We may conclude that the resonance interaction gives rise to an infinite number of periodic motions around the separatrix.

The map, Eq. (2.23), is essentially the same map as the whisker map which has been derived and discussed by Chirikov[18] in his study of a driven pendulum. Here we summarize his findings about the structure of the phase space (for $c'>0$).

(i) The fixed solutions given by Eq. (2.25) are all unstable at $\alpha=\pi\mu$. On the other hand, they are stable at $\alpha=0$ for $x>x_1$ and unstable for $x<x_1$, where

$$x_1 = \frac{w}{4\mu} . \tag{2.26}$$

Consequently, we have a region around the separatrix, $0 \le x < x_1$, where all fixed solutions are unstable. We may expect that the motion inside this region is very erratic.

(ii) Above the threshold value $x_1$ there is another threshold value which gives the boundary that separates the erratic motion from the regular motion. The value of $x_0$ is evaluated from the "overlapping criterion" of the resonance region; erratic motion begins to occur, if the separatrices surrounding adjacent stable fixed points touch. This value is given by

$$x_0 = \frac{w}{\mu} . \tag{2.27}$$

For $x_1 \le x < x_0$ the motion is still erratic because of the overlapping effect of the resonances. However, because there are stable fixed points in this region, we can observe some regular motion around these stable fixed points. In the Poincaré map we see a mixed structure of erratic points and islands of regular points.

Because trajectories cannot cross each other, the motion in the erratic region is confined to a thin layer, $|x| \le x_0$, around the separatrix. We call this layer the stochastic layer.

In each map the value of $y_2$ is also confined to a small region. This region can be easily estimated from the energy conservation for a given energy surface $H=E$ in the stochastic layer and is given by

$$|\sqrt{y_2}-\sqrt{y_{20}}| \lesssim \tfrac{5}{2}\lambda\mu , \tag{2.28}$$

where we have neglected higher-order terms of $\mu/\sqrt{y_2}$. The minimum value of $\sqrt{y_2}$ is given at $\alpha_1=0$, $\alpha_2=\mu\pi$; the maximum value at $\alpha_1=\alpha_2=0$.

We may estimate the average period of the pendulum $T_{c'}$, Eq. (2.11), in the stochastic layer such as

$$\bar{T} \equiv \frac{1}{c_0'}\int_0^{c_0'} T_{c'}dc' = \ln\left[\frac{16e}{c_0'}\right] \simeq \frac{\pi}{2\mu} , \tag{2.29}$$

where $c_0'=2x_0$. This shows that the system has two time scales well separated for sufficiently small $\mu$; one is the time scale for free motion, the order of which is given by $\bar{T}$, and the other is the interaction time $t_i$ the order of which is 1.

Similarly, we may estimate the average value of the discreteness of the spectrum of the Fourier component $\Delta k$ in Eq. (2.15) in the stochastic layer, which is given by $\overline{\Delta k} \simeq 2\mu$.

## III. KINETIC EQUATION IN THE STOCHASTIC LAYER

In this section we derive a kinetic equation which describes long-time behavior of the system in the stochastic layer. The method on which we rely here is the perturbation theory developed by Prigogine and his colleagues[4–7] for nonequilibrium statistical systems. When we apply this method to nonlinear systems, however, we need a few extensions of the perturbation theory such that we may treat systems the periodicity of which depends on the momentum. The extension will be pointed out in the following context of the derivation of the kinetic equation.

In order to describe the evolution of the system, we start with the Liouville equation

$$i\frac{\partial}{\partial t}\rho(\vec{\alpha},\vec{y},t)=L\rho(\vec{\alpha},\vec{y},t)\ . \tag{3.1}$$

Here, $\rho$ is the distribution function of the ensemble of the system in the stochastic layer and $\vec{\alpha}=(\alpha_1,\alpha_2)$ and $\vec{y}=(y_1,y_2)$ are abbreviations of the canonical variables with the vector notation. The function $\rho$ is normalized such that

$$\int_{y_m}^{y_M}dy_2\int_{1-x_0}^{1+x_0}dy_1\int_{-\pi/\Delta k_2}^{\pi/\Delta k_2}d\alpha_2\int_{-\pi/\Delta k_1}^{\pi/\Delta k_1}d\alpha_1\rho(\alpha_1,\alpha_2,y_1,y_2)=1\ , \tag{3.2}$$

where $y_M$ and $y_m$ are the upper and lower bounds of the values of $y_2$ satisfying $\mu \ll y_m < y_M \ll \mu^{-1}$ in the ensemble, $x_0$ is the boundary value of the stochastic layer given in Eq. (2.28) with $y_{20}=y_2$, $\Delta k_2=\mu^{-1}$, and

$$\Delta k_1=\begin{cases}\dfrac{\pi}{2K}, & c'\geq 0\\ \dfrac{\sqrt{c}\,\pi}{2K_-}, & c'<0\end{cases} \tag{3.3}$$

where $K_-\equiv K(c^{-1})$. Note that the domain of the integral of $\alpha_1$ depends on the momentum $y_1$ because of the nonlinearity of the system.

The operator $L$ is the Liouvillian which is defined by the Poisson bracket $L=i\{H,\ \}$ where the factor $i$ is introduced to make $L$ a Hermitian operator. Corresponding to the decomposition of the Hamiltonian, Eq. (2.4), we have the decomposition of $L$,

$$L=L_0+\lambda\,\delta L\ , \tag{3.4}$$

where

$$L_0=-i\vec{\omega}\cdot\frac{\partial}{\partial\vec{\alpha}}\ , \tag{3.5}$$

$$\lambda\,\delta L=i\lambda\left[\frac{\partial V}{\partial\vec{\alpha}}\cdot\frac{\partial}{\partial\vec{y}}-\frac{\partial V}{\partial\vec{y}}\cdot\frac{\partial}{\partial\vec{\alpha}}\right]\ , \tag{3.6}$$

and $\vec{\omega}=(\omega_1,\omega_2)=(\partial H_0/\partial y_1,\partial H_0/\partial y_2)=(2y_1,1)$, $\partial/\partial\vec{\alpha}=(\partial/\partial\alpha_1,\partial/\partial\alpha_2)$, and so on, and we have used the notation of the inner product, i.e., $\vec{A}\cdot\vec{B}=A_1B_1+A_2B_2$.

Because the unperturbed Liouvillian $L_0$ is simply a derivative operator of the coordinate, we may immediately solve the eigenvalue problem of $L_0$ and have

$$L_0\Phi_{k_1,k_2}(\alpha_1,\alpha_2)=(k_1\omega_1+k_2\omega_2)\Phi_{k_1,k_2}(\alpha_1,\alpha_2) \tag{3.7}$$

with the eigenfunction $\Phi_{k_1,k_2}$ given by

$$\Phi_{k_1,k_2}(\alpha_1,\alpha_2)=\frac{(\Delta k_1\,\Delta k_2)^{1/2}}{2\pi}e^{i(k_1\alpha_1+k_2\alpha_2)}\ . \tag{3.8}$$

Here $k_1=n\,\Delta k_1$ and $k_2=m\,\Delta k_2$ where $n$ and $m$ are any integers, and we have imposed periodic boundary conditions on the eigenfunction with period of $2\pi/\Delta k_1$ for $\alpha_1$ and $2\pi/\Delta k_2$ for $\alpha_2$, respectively.

The eigenfunction consists of a complete orthonormal set such that

$$\sum_{k_1}\sum_{k_2}\Phi_{k_1,k_2}(\alpha_1,\alpha_2)\Phi^*_{k_1,k_2}(\alpha_1',\alpha_2')=\delta(\alpha_1-\alpha_1')\delta(\alpha_2-\alpha_2')\ , \tag{3.9a}$$

$$\int_{-\pi/\Delta k_2}^{\pi/\Delta k_2}d\alpha_2\int_{-\pi/\Delta k_1}^{\pi/\Delta k_1}d\alpha_1\Phi^*_{k_1,k_2}(\alpha_1,\alpha_2)\Phi_{k_1',k_2'}(\alpha_1,\alpha_2)=\delta_{k_1,k_1'}\delta_{k_2,k_2'}\ , \tag{3.9b}$$

where the superscript asterisk denotes the complex conjugate, and $\sum_{k_2}\sum_{k_1}$ and $\delta_{k_1,k_1'}\delta_{k_2,k_2'}$ are abbreviations of $\sum_{m=-\infty}^{+\infty}\sum_{n=-\infty}^{+\infty}$ and $\delta_{n,n'}\delta_{m,m'}$, respectively, for $k_1=n\,\Delta k_1$ and $k_2=m\,\Delta k_2$. Sufficiently close to the separatrix, i.e., $\Delta k_1\ll 1$, the summation $\Delta k_1\sum_{k_1}$ reduces to the integration $\int_{-\infty}^{+\infty}dk_1$.

In order to make notation simpler in the following calculation, it is convenient to introduce a "Dirac" bra-ket notation. In this notation the eigenfuction $\Phi_{k_1,k_2}$ is represented as an inner product of bra and ket vectors by

$$\Phi_{k_1,k_2}(\alpha_1,\alpha_2)=\langle\vec{\alpha}\,|\,\vec{k}\rangle\ , \tag{3.10}$$

where $|\,\vec{k}\rangle=|\,k_1,k_2\rangle$ is the eigen-ket vector of $L_0$, i.e.,

$$L_0\,|\,\vec{k}\rangle=(\vec{k}\cdot\vec{\omega})\,|\,\vec{k}\rangle\ . \tag{3.11}$$

The complete orthonormality of the eigenvector is expressed by

$$\sum_{\vec{k}}|\,\vec{k}\rangle\langle\vec{k}\,|=1\ , \tag{3.12a}$$

$$\langle\vec{k}\,|\,\vec{k}'\rangle=\delta_{\vec{k},\vec{k}'}\ , \tag{3.12b}$$

where $\sum_{\vec{k}}=\sum_{k_1}\sum_{k_2}$ and $\delta_{\vec{k},\vec{k}'}=\delta_{k_1,k_1'}\delta_{k_2,k_2'}$.

We further introduce a certain matrix element defined by

$$\langle\vec{k}\,|L|\,\vec{k}'\rangle=\int_{-\pi/\Delta k_2}^{\pi/\Delta k_2}d\alpha_2\int_{-\pi/\Delta k_1}^{\pi/\Delta k_1}d\alpha_1\Phi^*_{k_1,k_2}(\alpha_1,\alpha_2)L\times\Phi_{k_1',k_2'}(\alpha_1,\alpha_2)\ . \tag{3.13}$$

Obviously, this expression is still an operator of the momenta with the derivative acting on everything to its right.

By the definition of $L$, we have

$$\langle\vec{k}\,|L_0|\,\vec{k}'\rangle=(\vec{k}\cdot\vec{\omega})\delta_{\vec{k},\vec{k}'} \tag{3.14}$$

and

$$\langle \vec{k} \mid \lambda\delta L \mid \vec{k}' \rangle = \lambda\sqrt{\Delta k_1}\left[-V_{\vec{k}-\vec{k}'}(\vec{k}-\vec{k}')\cdot\frac{\partial}{\partial\vec{y}} + \left[\frac{\partial}{\partial\vec{y}}\cdot\vec{k}'V_{\vec{k}-\vec{k}'}\right]\right]\sqrt{\Delta k_1} . \quad (3.15)$$

Here, $V_{\vec{k}}$ is the Fourier component of the interaction in the Hamiltonian, Eq. (2.13), i.e.,

$$\lambda V(\vec{\alpha},\vec{y}) = \lambda\,\Delta k_1 \sum_{\vec{k}} V_{\vec{k}}(\vec{y}) e^{i\vec{k}\cdot\vec{\alpha}} , \quad (3.16)$$

where

$$V_{\vec{k}}(\vec{y}) = u_{k_1}(y_1) v_{k_2}(y_2) \quad (3.17)$$

with

$$u_{k_1}(y_1) = \begin{cases} \dfrac{\mu y_1^2}{\Delta k_1}\left[2-c-\dfrac{6E}{K}\right]\delta_{k_1,0} - \dfrac{12\mu y_1^2 k_1}{\sinh(2k_1K')}(1-\delta_{k_1,0}) & \text{for } c'\geq 0 \quad (3.18a) \\ \dfrac{\mu y_1^2}{\Delta k_1}\left[2-c-6\left[\dfrac{cE_-}{K_-}+c'\right]\right]\delta_{k_1,0} - \dfrac{12\mu k_1}{\sinh(2k_1K_1')}(1-\delta_{k_1,0}) & \text{for } c'<0 \quad (3.18b) \end{cases}$$

where $E_- \equiv E(c^{-1})$, $K'_- \equiv K'(c^{-1})$, and so on, and

$$v_{k_2}(y_2) = \frac{\sqrt{y_2}}{2}(\delta_{m,1}+\delta_{m,-1}) \quad (3.19)$$

for $k_2 = m\Delta k_2$. Note that because of the nonlinearity of the system, $\Delta k_1$ and $k_1$ in Eq. (3.15) depend on the momentum $y_1$ and they cannot commute with the derivative operator $\partial/\partial y_1$.

To obtain the kinetic equation, we need to specify the class of the ensemble in phase space. In this paper we restrict the class such that the distribution function of the ensemble is expanded in the following Fourier series at time $t=0$:

$$\rho(\vec{\alpha},\vec{y}) = \frac{\Delta k_1 \Delta k_2}{(2\pi)^2}\sum_{k_2}\left[\rho_{0,k_2}(\vec{y}) + \Delta k_1 \sum_{k_1}{}'\rho_{k_1,k_2}(\vec{y})e^{ik_1\alpha_1}\right]e^{ik_2\alpha_2} . \quad (3.20)$$

Here, $\rho_{0,k_2}$ stands for the Fourier component having $k_1=0$, and $\rho_{k_1,k_2}$ for the component having $k_1\neq 0$. We assume that $\rho_{0,k_2}$ and $\rho_{k_1,k_2}$ in Eq. (3.20) have finite values in the limit of $\Delta k_1 \to 0$. This assumption is a direct extension of the assumption for the volume dependence of each Fourier component of the distribution function in a gaseous system enclosed in a large box, which has been made by Prigogine and Balescu.[4] The physical meaning of this assumption is that we consider only ensembles the distribution function of which depends smoothly on the coordinate $\alpha_1$ and the deviation of the distribution on $\alpha_1$ from the uniform distribution is not pathologically large.[23] (For more detailed discussion of this assumption, see Ref. 5).

Denoting the distribution function $\rho(\vec{\alpha},\vec{y})$ by the braket notation, such that

$$\rho(\vec{\alpha},\vec{y}) = \langle \vec{\alpha} \mid \rho \rangle = \sum_{\vec{k}} \langle \vec{\alpha} \mid \vec{k} \rangle \langle \vec{k} \mid \rho \rangle , \quad (3.21)$$

and comparing it with the expansion, Eq. (3.20), we obtain the relation

$$\rho_{0,k_2}(\vec{y}) = \frac{2\pi}{\sqrt{\Delta k_1 \Delta k_2}}\langle 0,k_2 \mid \rho \rangle \quad (3.22)$$

and a similar relation between $\rho_{k_1,k_2}$ and $\langle k_1,k_2 \mid \rho \rangle$.

Note that $\rho_{\vec{0}}(\vec{y}) \equiv \rho_{0,0}(\vec{y})$ is just the momentum distribution function,

$$\rho_{\vec{0}}(\vec{y}) = \int_{-\pi/\Delta k_2}^{\pi/\Delta k_2} d\alpha_2 \int_{-\pi/\Delta k_1}^{\pi/\Delta k_1} d\alpha_1 \rho(\vec{\alpha},\vec{y}) \quad (3.23)$$

which is an invariant of the motion in the unperturbed system.

In order to pick up dominant contributions in the long time scale in the perturbation series of the solution, we here introduce a projection operator $P$ which projects out the time-invariant component of a given phase function in the unperturbed system and also introduce its complementary projection operator $Q$, which are defined by

$$P = \mid \vec{0} \rangle \langle \vec{0} \mid , \quad Q = \sum_{\vec{k}}{}' \mid \vec{k} \rangle \langle \vec{k} \mid . \quad (3.24)$$

They are Hermitian operators and satisfy the following relations:

$$P+Q=1 , \quad P^2=P , \quad Q^2=Q , \quad PQ=QP=0 , \quad (3.25)$$

and

$$PL_0 = L_0P = 0 , \quad QL_0 = L_0Q . \quad (3.26)$$

Using these operators, we can decompose $\mid\rho\rangle$ into orthogonal components such that $\mid\rho\rangle = P\mid\rho\rangle + Q\mid\rho\rangle$: The component $Q\mid\rho\rangle$ is related to the geometrical configuration of the ensemble in the configuration space of the system. Following the terminology in nonequilibrium statistical mechanics,[5] we call this component the "correlation component" and the component $P\mid\rho\rangle$ the "vacuum of correlation component" (or, merely, vacuum component).

The formal solution of the Liouville equation is given by the resolvent operator of the Liouvillian $(z-L)^{-1}$ in a Laplace transform

$$|\rho(t)\rangle = e^{-iLt}|\rho(0)\rangle = \frac{1}{2\pi i}\int_\Gamma dz\, e^{-izt}\frac{1}{z-L}|\rho(0)\rangle \ , \tag{3.27}$$

where the contour $\Gamma$ lies above the real axis of $z$ and goes from $+\infty$ to $-\infty$ for $t>0$.

In the resolvent formalism in the perturbation theory, the asymptotic contribution of Eq. (3.27) for $t\to+\infty$ is estimated by evaluating the singularity of the integrand at $z=0$. To make this singularity explicit, we rewrite the resolvent operator by the following identity:

$$\frac{1}{z-L} = [P+\mathscr{C}(z)]\frac{1}{z-PLP-\psi(z)}[P+\mathscr{D}(z)]+\mathscr{P}(z) \ , \tag{3.28}$$

where

$$\psi(z) = PLQ\frac{1}{z-QLQ}QLP \ , \tag{3.29}$$

$$\mathscr{D}(z) = PLQ\frac{1}{z-QLQ} \ , \tag{3.30}$$

$$\mathscr{C}(z) = \frac{1}{z-QLQ}QLP \ , \tag{3.31}$$

and

$$\mathscr{P}(z) = \frac{1}{z-QLQ}Q \ . \tag{3.32}$$

The identity Eq. (3.28) can be proved by a simple algebraic manipulation with Eq. (3.25). The operators $\psi$, $\mathscr{D}$, $\mathscr{C}$, and $\mathscr{P}$, which we call kinetic operators, are basic quantities in our formalism. The operator $\psi$ is called the "collision operator" and it determines the evolution of $P|\rho(t)\rangle$ through an intermediate state in the $Q$ subspace. This operator is an extension of the collision kernel appearing in a kinetic equation (such as the Boltzmann equation in a dilute gas). The operator $\mathscr{D}(z)$ and $\mathscr{C}(z)$ are called the "destruction operator" and the "creation operator," respectively. The former describes the decay process of the initial spatial correlation, while the latter describes the creation process of a new correlation. The operator $\mathscr{P}(z)$ is called the "propagation operator," which describes the propagation process of the initial correlation in the $Q$ subspace. More details of these concepts are found in Ref. 5.

The decomposition of the resolvent operator, Eq. (3.28), is still formal, because we do not know the inverse operators of $z-QLQ$ and $z-PLP-\psi(z)$. We may, however, construct explicitly these operators by the perturbation expansion. For example, the collision operator is given by

$$\psi(z) = P\lambda\,\delta L\, Q\frac{1}{z-QL_0Q}\sum_{n=0}^{\infty}\left[Q\lambda\,\delta L\, Q\frac{1}{z-QL_0Q}\right]^n \times Q\lambda\,\delta L\, P \ , \tag{3.33}$$

where we have used the relations in Eq. (3.26). Note that the collision operator is defined in the perturbation series such that each term does not have the singularity at $z=0$ that comes from the $P$ subspace in the intermediate state of the perturbation expansion. Remaining kinetic operators are similarly constructed by the perturbation series, and they have the same properties on the singularity at $z=0$ with $\psi(z)$.

Because the Liouville is the Hermitian operator, the function obtained by operating the kinetic operators to a given function is analytic in the upper half-plane and the lower half-plane of $z$, except for the real axis. In the limit of the continuous spectrum of the unperturbed Liouvillian, i.e., $\Delta k_1\to 0$, each term in the perturbation series in Eq. (3.30) operating to a given function is expressed by a Cauchy integral and has a discontinuity on the real axis of $z$.[6] In this case, the integration of $z$ in Eq. (3.27) must be performed with analytically continued functions of the kinetic operators from the upper half-plane of $z$ to the lower half-plane for $t>0$.

Substituting Eq. (3.28) into (3.27) and expanding the factor including $\psi(z)$ in a series we obtain

$$P|\rho(t)\rangle = \frac{1}{2\pi i}\sum_{n=0}^{\infty}\int_\Gamma dz\, e^{-izt}\frac{1}{z^{n+1}}[\psi(z)]^n \times[P+\mathscr{D}(z)]|\rho(0)\rangle \tag{3.34}$$

and

$$Q|P(t)\rangle = \frac{1}{2\pi i}\sum_{n=0}^{\infty}\int_\Gamma dz\, e^{-izt} \times\left[\mathscr{C}(z)\frac{1}{z^{n+1}}[\psi(z)]^n[P+\mathscr{D}(z)] + \mathscr{P}(z)\right]|\rho(0)\rangle \ , \tag{3.35}$$

where we have used the relation $PLP=0$ which is obtained from Eqs. (3.14), (3.15), and the definition of $P$ in Eq. (3.24).

The asymptotic contributions of Eqs. (3.34) and (3.35) for $t\to+\infty$ are obtained by evaluating the singularities at $z=0$. To evaluate them, let us here assume that the singularities at $z=0$ of $z^{-(n+1)}$ in Eqs. (3.34) and (3.35) are isolated from the singularities of the analytically continued kinetic operators. For sufficiently small $\mu$ we can verify this assumption. (For this case, we will show later that the singularities of the kinetic operators are poles in the lower half-plane.) Thus we may neglect the contributions coming from the singularities of the kinetic operators for asymptotic time evolution. Evaluating the residue of the integrand at $z=0$ in Eqs. (3.34) and (3.35), we obtain the asymptotic solution for $t\to+\infty$,

$$P|\rho(t)\rangle = \sum_{n=0}^{\infty}\frac{1}{n!}\left[\frac{\partial^n}{\partial z^n}e^{-izt}[\psi(z)]^n \times[P+\mathscr{D}(z)]|\rho(0)\rangle\right]_{z=+i0} \tag{3.36}$$

and

$$Q\,|\rho(t)\rangle=\sum_{n=0}^{\infty}\frac{1}{n!}\left[\frac{\partial^n}{\partial z^n}e^{-izt}\mathscr{C}(z)[\psi(z)]^n \times[P+\mathscr{D}(z)]\,|\rho(0)\rangle\right]_{z=+i0}, \quad (3.37)$$

where $z=+i0$ means that the residue is taken for analytically continued kinetic operators from the upper half-plane of $z$.

Introducing the inverse Laplace transforms of the collision operator and the creation operator by

$$\psi(z)=i\int_0^{\infty}dt\,e^{izt}\tilde{\psi}(t) \quad (3.38)$$

and

$$\mathscr{C}(z)=i\int_0^{\infty}dt\,e^{izt}\tilde{\mathscr{C}}(t) \quad (3.39)$$

and using the Leibnitz formula for the derivative in Eqs. (3.36) and (3.37), we obtain the following asymptotic equations:

$$\frac{\partial}{\partial t}P\,|\rho(t)\rangle=\int_0^{\infty}dt'\tilde{\psi}(t')P\,|\rho(t-t')\rangle \quad (3.40)$$

and

$$Q\,|\rho(t)\rangle=i\int_0^{\infty}dt'\tilde{\mathscr{C}}(t')P\,|\rho(t-t')\rangle\ . \quad (3.41)$$

By introducing a new operator $\Theta$, Eq. (3.40) can be written in the following compact form:

$$i\frac{\partial}{\partial t}P\,|\rho(t)\rangle=\Theta P\,|\rho(t)\rangle\ . \quad (3.42)$$

Here, the equation for $\Theta$ is obtained by substituting the formal solution of Eq. (3.42), $P\,|\rho(t)\rangle=\exp(-i\Theta t)P\,|\rho(0)\rangle$, into both sides of Eq. (3.40) and we obtain

$$\Theta=\sum_{n=0}^{\infty}\frac{1}{n!}\left[\frac{\partial^n}{\partial z^n}\psi(z)\right]_{z=+i0}\Theta^n\ . \quad (3.43)$$

Similarly, introducing the new operator $C$ by

$$C=\sum_{n=0}^{\infty}\frac{1}{n!}\left[\frac{\partial^n}{\partial z^n}\mathscr{C}(z)\right]_{z=+i0}\Theta^n \quad (3.44)$$

we have an alternative expression of Eq. (3.41)

$$Q\,|\rho(t)\rangle=CP\,|\rho(t)\rangle\ . \quad (3.45)$$

This result shows that the $Q$ component of $|\rho(t)\rangle$ becomes a functional of the $P$ component in the asymptotic time limit.

From Eqs. (3.43) and (3.44), we can easily obtain the lowest-order approximation of $\Theta$ and $C$ with respect to $\lambda$ such that

$$\Theta\simeq\psi_2(+i0) \quad (3.46)$$

and

$$C\simeq\mathscr{C}_1(+i0)\ , \quad (3.47)$$

where $\psi_2(z)$ and $\mathscr{C}_1(z)$ are the lowest-order approximation of $\psi(z)$ and $\mathscr{C}(z)$ in Eqs. (3.29) and (3.31), respectively, and given by

$$\psi_2(z)=\lambda^2P\,\delta L\,Q\frac{1}{z-QL_0Q}Q\,\delta L\,P\ , \quad (3.48a)$$

which gives us

$$\langle\vec{0}\,|\,\psi_2(+i0)\,|\,\vec{0}\rangle=i\pi\lambda^2\sum_{\vec{k}}{}'\sqrt{\Delta k_1}\frac{\partial}{\partial\vec{y}}\cdot\vec{k}\,\Delta k_1\,|\,V_{\vec{k}}\,|^2 \times\delta(\vec{k}\cdot\vec{\omega})\vec{k}\cdot\frac{\partial}{\partial\vec{y}}\sqrt{\Delta k_1}\ , \quad (3.48b)$$

and

$$\mathscr{C}_1(z)=\lambda\frac{1}{z-QL_0Q}Q\,\delta L\,P \quad (3.49a)$$

which gives us

$$\langle\vec{k}\,|\,\mathscr{C}_1(+i0)\,|\,\vec{0}\rangle=\lim_{\epsilon\to0+}\left[\lambda\sqrt{\Delta k_1}\frac{V_{\vec{k}}}{(\vec{k}\cdot\vec{\omega})-i\epsilon}\vec{k}\cdot\frac{\partial}{\partial\vec{y}}\sqrt{\Delta k_1}\right]\ . \quad (3.49b)$$

Here we have used the Plomelj formula

$$\lim_{\epsilon\to0+}\frac{1}{x-i\epsilon}=\mathrm{P}\frac{1}{x}+i\pi\delta(x)\ , \quad (3.50)$$

where P stands for the principal part of $1/x$: the principal part in Eq. (3.41) does not contribute due to the symmetry of the function of $\vec{k}$. In Eq. (3.48b) we interpret the summation of $k_1$ as the integration of $k_1$, i.e., $\Delta k_1\sum_{k_1}\to\int dk_1$, since $\Delta k_1\ll1$ holds in the stochastic layer.

Combining all above results, we arrive at the lowest-order approximation of the asymptotic kinetic equations,

$$i\frac{\partial}{\partial t}\langle\vec{0}\,|\,\rho(t)\rangle=\langle\vec{0}\,|\,\psi_2(+i0)\,|\,\vec{0}\rangle\langle\vec{0}\,|\,\rho(t)\rangle \quad (3.51)$$

and

$$\langle\vec{k}\,|\,\rho(t)\rangle=\langle\vec{k}\,|\,\mathscr{C}_1(+i0)\,|\,\vec{0}\rangle\langle\vec{0}\,|\,\rho(t)\rangle\ , \quad (3.52)$$

or, equivalently,

$$\frac{\partial}{\partial t}\rho_{\vec{0}}(\vec{y},t)=\pi\lambda^2\sum_{\vec{k}}{}'\frac{\partial}{\partial\vec{y}}\cdot\vec{k}\,\Delta k_1\,|\,V_{\vec{k}}\,|^2 \times\delta(\vec{k}\cdot\vec{\omega})\vec{k}\cdot\frac{\partial}{\partial\vec{y}}\Delta k_1\rho_{\vec{0}}(\vec{y},t) \quad (3.53)$$

and

$$\rho_{0,k_2}(\vec{y},t)=\lim_{\epsilon\to0+}\left[\frac{\lambda V_{0,k_2}}{k_2\omega_2-i\epsilon}k_2\frac{\partial}{\partial y_2}\Delta k_1\rho_{\vec{0}}(\vec{y},t)\right]\ , \quad (3.54a)$$

$$\Delta k_1\rho_{k_1,k_2}(\vec{y},t)=\lim_{\epsilon\to0+}\left[\frac{\lambda V_{\vec{k}}}{(\vec{k}\cdot\vec{\omega})-i\epsilon}\vec{k}\cdot\frac{\partial}{\partial\vec{y}}\Delta k_1\rho_{\vec{0}}(\vec{y},t)\right]\ . \quad (3.54b)$$

Note that the right-hand side of Eq. (3.53) has a contribution only at the resonance point, $\vec{k}\cdot\vec{\omega}=0$. These results show a conspicuous distinction of our perturbation theory from others (e.g., the KAM theory), that is, our theory is applicable in the resonance region.

## IV. PROPERTIES OF THE KINETIC EQUATION AND EQUILIBRIUM STATE

In this section we show that the kinetic equation (3.53) reduces to a one-dimensional Fokker-Planck equation for a suitable choice of variables, and describes a motion of the system which approaches an equilibrium state. We also estimate the diffusion coefficient of the unperturbed energy of the pendulum in the stochastic layer, and compare our result with a result which is obtained by Chirikov's heuristic argument.

Let us replace the independent variables $(y_1,y_2)$ in the kinetic equation by $(y_1,H_0)$, where $H_0$ is the unperturbed energy, i.e., $H_0=y_1^2+y_2$. In the new variables, terms involving the derivative operator $\partial/\partial H_0$ in Eq. (3.53) vanish because of the relation $(\vec{k}\cdot\vec{\omega})\delta(\vec{k}\cdot\vec{\omega})=0$ and we obtain the following continuous equation:

$$\frac{\partial}{\partial t}\phi(y_1,H_0,t)+\frac{\partial}{\partial y_1}j(y_1,H_0,t)=0 . \tag{4.1}$$

Here we have put $\phi(y_1,H_0,t)=\rho_0(y_1,y_2,t)$ and introduced the probability current by

$$j(y_1,H_0,t)=-\tfrac{1}{2}D'(y_1,H_0)\frac{\partial}{\partial y_1}\Delta k_1\phi(y_1,H_0,t) , \tag{4.2}$$

where

$$D'(y_1,H_0)=2\pi\lambda^2\Delta k_1 \sum_{\vec{k}}{}' \, |k_1V_{\vec{k}}|^2\delta(\vec{k}\cdot\vec{\omega}) \simeq \frac{18\pi\lambda^2}{\mu^2}\frac{H_0-y_1^2}{y_1}e^{-\pi/\mu y_1} . \tag{4.3}$$

This result shows that the evolution of the momentum-distribution function for the weakly coupled system is essentially one-dimensional on a unperturbed energy surface.

Introducing a diffusion coefficient $D$ and the drift coefficient $F$ by

$$D(y_1,H_0)=\Delta k_1 D'(y_1,H_0) , \tag{4.4}$$

$$F(y_1,H_0)=\tfrac{1}{2}\Delta k_1\frac{\partial}{\partial y_1}D'(y_1,H_0) , \tag{4.5}$$

we can further rewrite the kinetic equation (4.1) in the following form of the Fokker-Planck equation:

$$\frac{\partial}{\partial t}\phi(y_1,t)=-\frac{\partial}{\partial y_1}[F(y_1)\phi(y_1,t)] +\frac{1}{2}\frac{\partial^2}{\partial y_1^2}[D(y_1)\phi(y_1,t)] , \tag{4.6}$$

where we have omitted the argument $H_0$ in order to emphasize the one-dimensionality of the equation and to make notation simpler.

In the new variables the collision operator has also a simpler form,

$$\langle\vec{0}\,|\,\psi_2(+i0)\,|\,\vec{0}\rangle=i\sqrt{\Delta k_1}\frac{\partial}{\partial y_1}\frac{D'(y_1,H_0)}{2}\frac{\partial}{\partial y_1}\sqrt{\Delta k_1} . \tag{4.7}$$

To investigate further the evolution governed by our kinetic equation, we need to specify the boundary condition of the distribution function. Because the stochastic layer is restricted and isolated in the region of $|x|\le x_0$, where $x_0$ is given by Eq. (2.27) with $y_{20}\simeq H_0-1$, we assume that the probability current, Eq. (4.2), vanishes at the boundary of the stochastic layer, $x=x_0$. This boundary condition enables us to show that the operator $-i\psi_2(+i0)$ is a Hermitian operator in a space of the functions of $y_1$, i.e.,

$$\int_{1-x_0}^{1+x_0}dy_1 f_m^*(y_1)[-i\langle\vec{0}\,|\,\psi_2(+i0)\,|\,\vec{0}\rangle f_n(y_1)] = \left[\int_{1-x_0}^{1+x_0}dy_1 f_n^*(y_1)[-i\langle\vec{0}\,|\,\psi_2(+i0)\,|\,\vec{0}\rangle f_m(y_1)]\right]^* , \tag{4.8}$$

where $f_m$ and $f_n$ are any integrable functions of $y_1$ which satisfy the above-mentioned boundary condition.

Since the collision operator, Eq. (4.7), involves only the derivative operator of $y_1$, it is clear that a steady solution of Eq. (3.51) is given by

$$\langle\vec{0}\,|\,\rho_{\rm eq}\rangle=\frac{f_{\rm eq}(H_0)}{\sqrt{\Delta k_1}} , \tag{4.9}$$

where $f_{\rm eq}$ is any function of $H_0$.

We can further show that this steady solution is unique as a continuous function of $y_1$, and the distribution function $\langle\vec{0}\,|\,\rho(t)\rangle$ approaches this steady state monotonically, as follows. Let $\phi_i(y_1)$ be an eigenfunction of the operator $-i\psi_2(+i0)$ belonging to an eigenvalue $\lambda_i$ and satisfying the above-mentioned boundary condition. Since $-i\psi_2(+i0)$ is a Hermitian operator, we may assume that the eigenfunctions $\phi_i(y_1)$ consist of a complete orthonormal set. Then we have

$$\lambda_i=\int_{1-x_0}^{1+x_0}dy_1\phi_i^*(y_1)[-i\langle\vec{0}\,|\,\psi_2(+i0)\,|\,\vec{0}\rangle\phi_i(y_1)] =-\int_{1-x_0}^{1+x_0}dy_1\frac{D'(y_1,H_0)}{2}\left|\frac{\partial}{\partial y_1}\sqrt{\Delta k_1}\phi_i(y_1)\right|^2\le 0 . \tag{4.10}$$

Because the solution of Eq. (3.51) is expressed by $\langle\vec{0}\,|\,\rho(t)\rangle=\exp[-i\langle\vec{0}\,|\,\psi_2(+i0)\,|\,\vec{0}\rangle t]\langle\vec{0}\,|\,\rho(0)\rangle$, the result, Eq. (4.10), implies that the state belonging to $\lambda_i$ approaches zero monotonically, except for the state belonging to $\lambda_i=0$ which gives us the equilibrium state, Eq. (4.9).

Combining the result, Eq. (4.9), with the relations (3.20) and (3.54), we can calculate the equilibrium solution of the full distribution function $\rho_{\rm eq}(\vec{\alpha},\vec{y})$ and obtain

$$\rho_{\rm eq}(\vec{\alpha},\vec{y})=F_{\rm eq}(H_0)+\lambda V(\vec{\alpha},\vec{y})\frac{d}{dH_0}F_{\rm eq}(H_0) , \tag{4.11}$$

where $F_{eq}(H_0)=(\sqrt{\Delta k_2}/2\pi)f_{eq}(H_0)$. The right-hand side of Eq. (4.11) is just the first two terms in the Taylor-series expansion of $F_{eq}(H)=F_{eq}(H_0+\lambda V)$ by $\lambda$. This implies that the equilibrium state is a microcanonical distribution for a given energy $H=E$.

To compare our result with a result obtained by Chirikov's heuristic argument,[18] let us rewrite the Fokker-Planck equation for the momentum $y_1$ to the equation for the energy of the unperturbed pendulum $H_1=y_1^2$. Because $|y_1-1|\ll 1$, we have $\partial/\partial y_1 \simeq 2\partial/\partial H_1$. Substituting it into Eq. (4.6), we obtain

$$\frac{\partial\phi}{\partial t}=-\frac{\partial}{\partial H_1}(F_{H_1}\phi)+\frac{1}{2}\frac{\partial^2}{\partial H_1^2}(D_{H_1}\phi)\ . \tag{4.12}$$

Here, the diffusion coefficient $D_{H_1}$ of $H_1$ is related to the one of $y_1$ in Eq. (4.4) by

$$D_{H_1}=4D(y_1,H_0)\simeq 72\pi\lambda^2\frac{H_0-y_1^2}{\mu^2 y_1}e^{-\pi/\mu y_1}\Delta k_1 \tag{4.13}$$

which is equivalent to Eq. (1.1), and the drift coefficient $F_{H_1}$ by

$$F_{H_1}=4F(y_1,H_0)\simeq 36\pi^2\lambda^2\frac{H_0-y_1^2}{\mu^3 y_1^2}e^{-\pi/\mu y_1}\Delta k_1\ . \tag{4.14}$$

This gives us

$$\frac{F_{H_1}^2}{D_{H_1}}=18\pi^3\lambda^2\frac{H_0-y_1^2}{\mu^4 y_1^3}e^{-\pi/\mu y_1}\Delta k_1\ll 1\ . \tag{4.15}$$

This implies that the drift process in the stochastic layer is negligible as compared with the diffusion process.

We now compare this result with the "diffusion coefficient" $D_{Ch}$ defined by Chirikov[18] such that

$$D_{Ch}=\frac{\langle[\Delta H_1]^2\rangle_{av}}{T_a}\simeq 2\times 12^2\pi\lambda^2 y_{20}\frac{e^{-\pi/\mu}}{\mu}\left\langle\sin^2\frac{\alpha}{\mu}\right\rangle_{av}$$
$$=12^2\pi\lambda^2 y_{20}\frac{e^{-\pi/\mu}}{\mu}\ . \tag{4.16}$$

Here $\Delta H_1\simeq 2\Delta y_1$ [cf. Eq. (2.20)] and $\bar{T}$ is given by Eq. (2.29). The quantity $\langle\sin^2(\alpha/\mu)\rangle_{av}$ stands for the ensemble average of $\sin^2(\alpha/\mu)$ with the equilibrium distribution function given by Eq. (4.11).

On the other hand, if we approximate, in Eq. (4.13), $y_1$ by 1 and $\Delta k_1$ by its average value in the stochastic layer, i.e., $\overline{\Delta k}_1=2\mu$, we have $D_{Ch}=D_{H_1}$. This shows that our kinetic equation describes essentially the same diffusion process which has been investigated by Chirikov with numerical computation.

Let us make a comment here on Chirikov's derivation of the diffusion coefficient. In his heuristic argument, he has assumed a uniform random phase distribution of the phase of the external field.[18] However, it is clear that the random phase distribution of the spring in our system is not compatible with the microcanonical one because of the existence of the gravitational field. That the nonuniformity of the distribution in $\alpha_2$ is due to the gravitational field may be seen by observing that the interaction term in Eq. (2.14) vanishes if $6\,\mathrm{sech}^2(\alpha_1/2)-1=6\cos^2(\theta_1/2)-1=0$ for $|c'|\ll 1$. Consequently at this angle $\theta_1$ the microcanonical distribution function is independent of $\alpha_2$ and therefore the spring "feels" space to be uniform. It is easily seen that at this angle the centrifugal force cancels the radial component of the gravitational force acting on the mass.

Finally, let us verify our assumption stated in obtaining Eqs. (3.36) and (3.37) that the singularities at $z=0$ of $z^{-(n+1)}$ in Eqs. (3.34) and (3.35) are isolated from the singularities of the analytically continued kinetic operators for sufficiently small $\mu$. We consider first the case of the collision operator $\psi_2(z)$ in Eq. (3.48b). Using the product expansion

$$\frac{\sinh(\pi x)}{\pi x}=\prod_{n=1}^{\infty}\left[1+\frac{x^2}{n^2}\right] \tag{4.17}$$

we can perform the integration of the Fourier argument $k$ in $\psi_2(z)$. Then we see that $\psi_2(z)$ has simple and double poles in the lower half-plane of $z$ at

$$z=\begin{cases}\pm\dfrac{1}{\mu}-i\dfrac{n\pi y_1}{K'}\ , & c'\geq 0\\[2ex] \pm\dfrac{1}{\mu}-i\dfrac{n\pi y_1}{K'_-}\ , & c'<0\end{cases} \tag{4.18}$$

where $n$ is taken over all positive integers. Therefore, $\psi_2(z)$ has no singularity in the neighborhood of $z=0$.

For the case of remaining kinetic operators $\mathscr{D}(z)$, $\mathscr{C}(z)$, and $\mathscr{P}(z)$, we need to restrict the initial state and observables such that their Fourier coefficients do not introduce a singularity at $z=0$ in the integration of the Fourier argument. Assuming this initial condition and these observables, we obtain a similar result to the one in the collision operator.

The result, Eq. (4.18), gives us also a time scale of the duration of the interaction, $t_i$, between the two degrees of freedom in a collision, since the effect of the interaction damps with the ratio of $[|\mathrm{Im}(z)|]^{-1}$. Then this gives us $t_i\simeq\frac{1}{2}$, the order of which coincides with $t_i\simeq 1$ which has been roughly estimated in getting Eq. (2.20).

## V. SUMMARY AND CONCLUDING REMARKS

With the extension of Prigogine's perturbation theory we have derived the kinetic equation of the Fokker-Planck type in the vicinity of the separatrix in the elastic pendulum with two degrees of freedom. The important step in obtaining the irreversible equation (that is, the nonvanishing collision operator) was the replacement of the summation of $k_1$ in Eq. (3.48b) by its integration. Indeed, the contribution from the $\delta$ function in the collision operator, Eq. (3.48b), exists only when the spectrum of the Liouvillian is continuous.

We have also shown that for a given energy the system approaches the microcanonical distribution monotonically. To get this result, we have assumed that our kinetic equation is valid in the whole region of the stochastic layer. Of course, this assumption is not valid because the islands found in the stochastic layer induce regular motion. However, we expect that the effect of the islands is only significant near the boundary of the stochastic layer.

The diffusion coefficient obtained from our kinetic equation has shown good agreement with the one obtained by Chirikov's heuristic argument. This result lends support to the validity of our discussion, since Chirikov's estimate has been tested by numerical simulation.[24]

Let us remark upon an analogy of characteristic time scales in the elastic pendulum to the ones in a dilute gas system with a short-range interaction. The order of the duration of the interation between the pendulum and the spring, $t_i$, is unity. We may regard $t_i$ as being analogous to the collision time in a dilute gas. Similarly, we may regard the mean period of the pendulum in the stochastic layer $t_m \simeq \pi/2\mu$ as being analogous to the mean free time. The largest time scale in our system is the time describing its relaxation to an equilibrium distribution $t_R$. For the case of the reflecting boundary which we have assumed, $t_R$ may be approximated by a mean approaching time to the boundary by the diffusion process, starting from the middle of the stochastic layer. From this we obtain $t_R \sim c_0'^2/D_{H_1} \sim \mu^{-3}$. In our system there is another time scale which does not have an analog in the dilute gas system, namely, the period of the uncoupled spring, $t_s = 2\pi\mu$. In the weak-coupling limit we may summarize these results in the following inequality:

$$t_s \ll t_i \ll t_m \ll t_R . \tag{5.1}$$

We note here that the existence of well-separated time scales is enumerated as one of the grounds to obtain a kinetic equation of the Markovian type in phenomenological arguments.[7]

The diffusion process described by our kinetic equation is very slow. (Note that the diffusion coefficient is exponentially small in the limit $\mu \rightarrow 0$.) This slowness is the result of the existence of the essential singularity of the interaction at $\mu = 0$. Even though it is very slow, our results suggests that an embryo of the irreversibility already exists in nonintegrable conservative systems with two degrees of freedom. Extension of our perturbation calculation to higher-order approximation will be given in forthcoming papers.

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## APPENDIX

In this appendix we show the relation of the action-angle variables $(j,\beta)$ of the unperturbed pendulum to the canonical variables $(y_1,\alpha_1)$ introduced in Eq. (2.7). Here we discuss only the case of the rotational motion. The librational case can be treated similarly.

The action variable $j$ is defined by

$$j = \frac{1}{2\pi}\oint d\theta_1 Y_1 = \frac{2}{\pi}\frac{E(c)}{\sqrt{c}} , \tag{A1}$$

where $c = 1/H_1$. This shows that the Hamiltonian $H_1$ depends only on the action variable, namely, the angle $\beta$ is a cyclic variable.

The generating function of the canonical transformation between $(Y_1,\theta_1)$ and $(j,\beta)$ is given by

$$W(j,\theta_1) = \frac{2}{\sqrt{c}} E\left[\frac{\theta_1}{2}, c\right] , \tag{A2}$$

where $E(X,c)$ is the elliptic integral of the second kind. The angle variable is given by

$$\beta = \frac{\partial W(j,\theta_1)}{\partial j} = \frac{\pi}{K(c)} F\left[\frac{\theta_1}{2}, c\right] , \tag{A3}$$

where $F(X,c)$ is the elliptic integral of the first kind.

Inverting Eqs. (A1) and (A3) we obtain the canonical transformation

$$\sin\frac{\theta_1}{2} = \pm \mathrm{sn}\left[\frac{K(c)}{\pi}\beta, c\right] , \qquad Y_1 = \pm\frac{1}{\sqrt{c}}\mathrm{dn}\left[\frac{K(c)}{\pi}\beta, c\right] . \tag{A4}$$

Comparing Eq. (A4) with Eq. (2.7a), we obtain our desired canonical transformation

$$\alpha_1 = \frac{K(c)}{2\pi}\beta , \quad y_1 = \frac{1}{\sqrt{c}} , \tag{A5}$$

where $c$ is related to $j$ by Eq. (A1). The inverse relation is given by

$$\beta = \frac{2\pi}{K(c)}\alpha_1 , \quad j = \frac{2}{\pi}\frac{E(c)}{\sqrt{c}} , \tag{A6}$$

where $c = 1/y_1^2$.

Note that the canonical transformation, Eq. (A4), is not defined at the separatrix, i.e., $c = 1$, while our transformation, Eq. (2.7a), is well-defined there. It is interesting to note that the relation between $\alpha_1$ and $\beta$ is essentially the same as the relation between the arguments of the Jacobi elliptic functions and the elliptic theta function.

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[23]A counterexample of this assumption is the distribution function corresponding to a trajectory which is expressed by the $\delta$ function. From our argument, we omit such an interesting but singular distribution function.
[24]Chirikov's estimate was tested for the whisker map by numerical simulation.[18] The author and Dr. J. Tennyson also tested the result, Eq. (4.13), by integrating the equation of motion with the Hamiltonian Eq. (2.4) by numerical simulation. The result showed a good agreement between the theory and the numerical calculation. We will publish this result elsewhere.