Chaos and nonunitary evolution in nonintegrable Hamiltonian systems

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The Hamilton-Jacobi canonical transformation theory is extended to treat nonintegrable Hamiltonian systems with a continuous Fourier spectrum. By a natural analytic continuation of the Fourier variable to the complex plane, a nonunitary operator for the canonical transformation is obtained. We apply this transformation to describe Chirikov's diffusion process near a separatrix in nonlinear systems with two degrees of freedom. Our formalism shows a clear distinction between the irreversible evolution of an ensemble with a finite measure from the reversible evolution of a trajectory in nonintegrable systems with chaotic motion. The condition for obtaining the irreversible kinetic equation in Hamiltonian systems is connected to the condition for the existence of homoclinic points around the separatrix. We also show that Prigogine's dissipativity condition in nonequilibrium statistical systems is equivalent to the nonintegrability condition for nonlinear systems with a few degrees of freedom.

I. INTRODUCTION

We have studied in a previous paper[1] the derivation of an irreversible kinetic equation which describes Chirikov's diffusion process[2] near a separatrix in a nonlinear Hamiltonian system with two degrees of freedom. The derivation has been done using asymptotic perturbation theory where we have collected the contributions, coming from the resonance effect, which give the most diverging terms in the asymptotic time limit $t \rightarrow \infty$. Asymptotic perturbation theory was first introduced by Van Hove,[3] where he derived a quantum kinetic equation for a system with an infinite number of degrees of freedom. Then, this theory was extensively developed by Prigogine and his colleagues[4–7] for quantum and classical nonequilibrium statistical systems. One of the main results of their development is that they could clearly distinguish the role of dynamics in the evolution of the system from the role of statistics. The statistical assumption involved in their theory was imposed only on the initial conditions. In his discussion, Prigogine[5] summarized a dynamical condition for irreversibility as the "dissipativity condition," that is, the "condition of the existence of nonvanishing collision operator." In spite of some remarkably successful applications,[6] however, there were still unclear aspects of their asymptotic perturbation theory in the following sense: If there are truly irreversible processes in Hamiltonian systems, then why does one need the asymptotic argument to derive the irreversible kinetic equation? What is the relation between the irreversible evolution in an ensemble of the system described by the Liouvillian formalism and the reversible evolution of a trajectory described by the Hamiltonian formalism? These questions also arise in our derivation of the irreversible kinetic equation in the nonlinear dynamical system with two degrees of freedom.[1]

To answer these questions for infinitely large systems, Prigogine and his colleagues[8,9] have developed a transformation theory by constructing a nonunitary operator which transforms the evolution operator with a group property to a new evolution operator with a semigroup property. In contrast to the asymptotic perturbation theory, the nonunitary transformation is not restricted to the long-time limit for describing the evolution of the system. Their idea to construct the transformation operator is the following.[9] First the concept of "correlation" as a Fourier component of the distribution function with respect to the coordinates is introduced. Then, from a formal solution of the Liouville equation in a perturbation analysis, a projection operator Π_k associated with a Fourier variable k is constructed, which projects a component of the distribution function the evolution of which is governed, independently of another correlation component, by the "subdynamics." In constructing Π_k, however, if there is a continuous spectrum of k, then there exists an ambiguity in analytic continuation of k into the complex variable. To remove the ambiguity, George[10] has introduced a mathematical prescription of the analytic continuation which is called the "$i\varepsilon$ rule." This rule is similar to the analytic continuation in scattering theory in quantum mechanics, but much more involved. Then, solving the operator equation $\Pi_k = \Lambda P_k \Lambda^{-1}$, where P_k is a projection operator which projects an eigenstate of the unperturbed Liouvillian, they determine the transformation operator Λ. Due to the $i\varepsilon$ rule, Λ is not a unitary operator. The nonunitarity gives the irreversible evolution of the system.

The purpose of this paper is to construct a similar nonunitary transformation operator for the nonintegrable Hamiltonian system with a few degrees of freedom. We may summarize our results in the following three statements.

(i) The nonunitary transformation theory can be interpreted as a natural extension of the Hamilton-Jacobi canonical transformation theory to systems with the continuous Fourier spectrum.

(ii) Reversible evolution of a trajectory in the nonintegrable Hamiltonian system does not contradict the irreversible evolution of an ensemble of the system whose distribution function in phase space satisfies a certain natural condition.

(iii) Prigogine's dissipativity condition is equivalent to the nonintegrability condition for systems which have homoclinic points in phase space.

In this paper, we do not directly follow the method of the construction of the nonunitary operator given by Prigogine *et al.*[9] Our method is more straightforward and makes the physical meaning of the $i\varepsilon$ rule clear, at least in the nonintegrable system with a few degrees of freedom. To obtain the transformation operator, we first reconstruct the Hamilton-Jacobi canonical transformation theory in terms of the Lie-algebraic formalism.[11–13] Then we construct, by a perturbation analysis, a canonical transformation operator which makes the given Hamiltonian cyclic. As is well known, the generating function of the canonical transformation has the "small denominator." The small denominator introduces a serious difficulty in the ordinary perturbation theory, when the system has a discrete Fourier spectrum. However, we point out that if the system has a continuous Fourier spectrum, then the Fourier series with the small denominator reduces to the Fourier integral with the form of the Cauchy integral[6] which is evaluated on the real axis. Here is a crucial part of our formulation. Note that for a suitable analytic continuation the Cauchy integral becomes well defined, in contrast to the Fourier series, so that there is no difficulty of the small denominator. To determine the branch of the analytic continuation, we impose a physical boundary condition to the evolution of the system. Then, we obtain the well-defined transformation operator that we want to construct.

In order to make the physical meaning of our boundary condition clear, we consider a nonintegrable system which has homoclinic points in phase space around the separatrix of the unperturbed integrable system. Examples of the system are given in Sec. IV. There, we will show that the Fourier spectrum is continuous in the limit of approaching the separatrix. When we investigate the evolution in this system, we must distinguish between two extremely different cases: one is the evolution of the trajectory and the other is the evolution of the ensemble, the distribution of which has a "δ-function singularity" in its Fourier representation. In the first case, we impose the boundary condition that the transformation operator generates the motion of the trajectory on the unstable manifold. We will see that this boundary condition has a close analogy with determining the solution as the incoming plane wave in scattering theory in quantum mechanics. Then, this condition gives a unique analytic continuation of certain matrix elements of the transformation operator at least in the lowest-order approximation in the perturbation theory. In this case, we do not see any irreversible processes in the evolution.

The second case is another crucial part of our formulation. The importance of the existence of the δ-function singularity in the distribution function in obtaining irreversible kinetic equations for systems with an infinite number of degrees of freedom was first pointed out by Prigogine and Balescu.[4] In Sec. V we will show that for our nonintegrable system this corresponds to the case that we choose the initial ensemble such that its distribution function contains a homoclinic point with a finite measure, such as the step function. The measure may become as small as we wish. Because of the δ-function singularity the Fourier component of the distribution with zero Fourier argument plays a distinctive role, in contrast to the case of the trajectory where this component is negligibly small in the Fourier integral. In this case, we impose the physical boundary condition that the Fourier component with zero Fourier argument approaches the steady solution in the limit $t \rightarrow +\infty$. This boundary condition determines the analytic continuation of the remaining matrix elements of the transformation operator which were not determined by the boundary condition which was imposed in the case of the trajectory. Combining both cases, we are able to determine every matrix element of the transformation operator. The form of the transformation operator obtained by this method coincides with the one obtained by the use of the $i\varepsilon$ rule, at least in the lowest-order approximation from the perturbation analysis. Applying this transformation operator to the Liouville equation, we will derive correctly the same kinetic equation for Chirikov's diffusion process which was obtained by the asymptotic perturbation theory in the previous paper.[1]

An interesting observation of our result is that because of the second boundary condition, the generating function of the transformation operator does not reduce to a single function, in contrast to the ordinary canonical transformation. Owing to this fact, the transformation operator is not a unitary operator, but a "star-unitary" operator, the concept of which was introduced by Prigogine *et al.*[9] to discuss the origin of irreversibility for infinitely large conservative systems.

We further note that if the transformation operator acts on the distribution function of the trajectory, then we can neglect the contribution from the matrix elements obtained from the second boundary condition. This means we cannot distinguish our transformation operator from the ordinary unitary operator in the evolution of the trajectory. In this sense, the reversible evolution of the trajectory does not contradict the irreversible evolution of the ensemble of the system. Because infinitely many homoclinic points are distributed in a very complicated fashion around the hyperbolic fixed point, it seems to us almost impossible to construct a distribution function which does not have the δ-function singularity, except for a preparation with infinite accuracy such as the distribution function for a single trajectory.

In our formulation, the existence of the homoclinic point is essential to obtain the irreversible kinetic equation. On the other hand, the existence of the homoclinic point in nonlinear Hamiltonian systems with a few degrees of freedom implies that the system is nonintegrable.[14,15] In the last section, we will show by constructing the Melnikov function[15,16] that Prigogine's dissipativity condition is equivalent to the nonintegrability condition in the nonlinear system which we address in this paper.

II. CANONICAL TRANSFORMATION OPERATOR

The Lie derivative L_F generated by a function $F(\mathbf{q},\mathbf{p})$ is defined by its action on an arbitrary function $f(\mathbf{q},\mathbf{p})$ such that

$$L_F f = i\{F,f\} , \tag{2.1}$$

where $\mathbf{q} \equiv (q_1, q_2, \ldots, q_N)$, $\mathbf{p} \equiv (p_1, p_2, \ldots, p_N)$, and $\{F,f\}$ is the Poisson bracket of F and f. In a phase space of dimension $2N$,

$$L_F = i \sum_{i=1}^{N} \left[\frac{\partial F}{\partial q_i}\frac{\partial}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial}{\partial q_i} \right] . \tag{2.2}$$

Suppose that F also depends on some parameter g (such as a coupling constant) so that $F \equiv F(\mathbf{q},\mathbf{p};g)$. Then the canonical transformation operator Λ_F which gives $(\mathbf{q},\mathbf{p}) \Longrightarrow (\mathbf{Q},\mathbf{P})$ by $\mathbf{Q} = \Lambda_F \mathbf{q}$ and $\mathbf{P} = \Lambda_F \mathbf{p}$ is defined as a solution of the operator equation[11–13]

$$-i \frac{\partial \Lambda_F}{\partial g} = L_F \Lambda_F , \tag{2.3}$$

with the initial condition

$$\Lambda_F(g=0) = 1 . \tag{2.4}$$

The inverse operator Λ_F^{-1} satisfies the equation

$$i \frac{\partial \Lambda_F^{-1}}{\partial g} = \Lambda_F^{-1} L_F \tag{2.5}$$

with

$$\Lambda_F^{-1}(g=0) = 1 . \tag{2.6}$$

Equations (2.3) and (2.5) have the formal solutions

$$\Lambda_F = 1 + i \int_0^g dg_1\, L_F(g_1) + i^2 \int_0^g dg_1 \int_0^{g_1} dg_2\, L_F(g_1) L_F(g_2) + \cdots , \tag{2.7a}$$

$$\Lambda_F^{-1} = 1 - i \int_0^g dg_1\, L_F(g_1) + (-i)^2 \int_0^g dg_1 \int_0^{g_1} dg_2\, L_F(g_1) L_F(g_2) + \cdots . \tag{2.7b}$$

Let us now specify the generating function F such that the operator Λ_F makes a given Hamiltonian $H(\mathbf{q},\mathbf{p};g)$ cyclic in the form

$$\Lambda_F^{-1} H(\mathbf{q},\mathbf{p};g) = \widetilde{H}(\mathbf{p};g) . \tag{2.8}$$

We assume that the Hamiltonian H consists of the unperturbed part H_0 and the perturbation gV of the form

$$H(\mathbf{q},\mathbf{p};g) = H_0(\mathbf{p}) + gV(\mathbf{q},\mathbf{p}) = H_0(\mathbf{p}) + g\,\Delta k \sum_{\mathbf{k}} V_{\mathbf{k}}(\mathbf{p}) e^{i\mathbf{k}\cdot\mathbf{q}} , \tag{2.9}$$

where $\Delta k = \Delta k_1, \Delta k_2, \ldots, \Delta k_N$, $k_i = n_i\, \Delta k_i$ with integer n_i and $\mathbf{k}\cdot\mathbf{q} = k_1 q_1 + k_2 q_2 + \cdots + k_N q_N$. In other words, we have assumed that the perturbation depends periodically on q_i with period $2\pi/\Delta k_i$ for $i = 1, \ldots, N$. The period generally depends on the momentum $\mathbf{p}$, and that some of the periods can become infinite for certain values of $\mathbf{p}$. We further assume that the coupling constant g is very small so that we can expand F and $\widetilde{H}$ in power series

$$F(\mathbf{q},\mathbf{p};g) = \sum_{n=0}^{\infty} g^n F_{n+1}(\mathbf{q},\mathbf{p}) , \tag{2.10}$$

$$\widetilde{H}(\mathbf{p};g) = \sum_{n=0}^{\infty} g^n H_n(\mathbf{p}) . \tag{2.11}$$

Then, Eqs. (2.7) give

$$\Lambda_F = 1 + igL_1 + \tfrac{1}{2} g^2 [(iL_1)^2 + iL_2] + \cdots , \tag{2.12a}$$

$$\Lambda_F^{-1} = 1 - igL_1 + \tfrac{1}{2} g^2 [(-iL_1)^2 - iL_2] + \cdots , \tag{2.12b}$$

where $L_1 = L_{F_1}$, $L_2 = L_{F_2}$, etc. Substituting Eqs. (2.10)–(2.12) into (2.8), we obtain

$$\begin{aligned} &-iL_1 H_0 + V = H_1 , \\ &-iL_2 H_0 + \tfrac{1}{2}[(-iL_1)^2 H_0 - 2iL_1 V] = 2H_2 , \end{aligned} \tag{2.13}$$

and so on.

Because the above formalism and the following argument for the time evolution of the Liouville equation have a close analogy with the formulation of quantum mechanics, it is convenient to introduce a "Dirac bra-ket" notation. In this notation, any periodic function of $\mathbf{q}$ is represented as an inner product of abstract bra and ket vectors in a Hilbert space

$$f(\mathbf{q}) = \langle \mathbf{q} \,|\, f \rangle . \tag{2.14}$$

The momentum $\mathbf{p}$ is regarded as a parameter. Then, the complete orthonormal basis of the Fourier expansion in Eq. (2.9) is represented by

$$\langle \mathbf{q} \,|\, \mathbf{k} \rangle = \left[\frac{\Delta k}{(2\pi)^N} \right]^{1/2} e^{i\mathbf{k}\cdot\mathbf{q}} . \tag{2.15}$$

The complete orthonormality is expressed in terms of the projection operator $P_{\mathbf{k}} \equiv |\mathbf{k}\rangle\langle\mathbf{k}|$ as

$$\sum_{\mathbf{k}} P_{\mathbf{k}} = 1 , \tag{2.16a}$$

$$P_{\mathbf{k}} P_{\mathbf{k}'} = P_{\mathbf{k}} \delta_{\mathbf{k},\mathbf{k}'} , \tag{2.16b}$$

where $\delta_{\mathbf{k},\mathbf{k}'} = \delta_{k_1,k_1'} \delta_{k_2,k_2'} \times \cdots \times \delta_{k_N,k_N'}$.

The matrix element of the Lie derivative is introduced by

$$\langle \mathbf{k} \,|\, L_F \,|\, \mathbf{k}' \rangle = \frac{\Delta k}{(2\pi)^N} \int_{-\pi/\Delta k_1}^{\pi/\Delta k_1} dq_1 \cdots \int_{-\pi/\Delta k_N}^{\pi/\Delta k_N} dq_N\, e^{-i\mathbf{k}\cdot\mathbf{q}} L_F e^{i\mathbf{k}'\cdot\mathbf{q}} . \tag{2.17}$$

Let us assume that the generating function F is expanded as a Fourier series

$$F(\mathbf{q},\mathbf{p})=\Delta k \sum_{\mathbf{k}}{}' F_{\mathbf{k}}(\mathbf{p})e^{i\mathbf{k}\cdot\mathbf{q}} , \tag{2.18}$$

where the prime on the summation sign stands for $\mathbf{k}\neq\mathbf{0}$. Then, we have

$$\langle \mathbf{k} \mid L_F \mid \mathbf{k}' \rangle = \sqrt{\Delta k}\left[-F_{\mathbf{k}-\mathbf{k}'}(\mathbf{k}-\mathbf{k}')\cdot\frac{\partial}{\partial \mathbf{p}} + \left[\frac{\partial}{\partial \mathbf{p}}\cdot\mathbf{k}'F_{\mathbf{k}-\mathbf{k}'}\right]\right]\sqrt{\Delta k} , \tag{2.19}$$

where $\mathbf{k}\cdot(\partial/\partial\mathbf{p})=k_1\partial/\partial p_1+k_2\partial/\partial p_2+\cdots+k_N\partial/\partial p_N$.

We now apply the Dirac notation to solve Eq. (2.13). From the first equation we obtain

$$-i\langle \mathbf{k} \mid L_1 \mid \mathbf{0}\rangle\langle \mathbf{0} \mid H_0\rangle+\langle \mathbf{k} \mid V\rangle=\langle \mathbf{k} \mid H_1\rangle\delta_{\mathbf{k},0} , \tag{2.20}$$

where $\langle \mathbf{0} \mid H_0 \rangle=(2\pi)^{N/2}(\Delta k)^{-1/2}H_0(\mathbf{p})$ and $\langle \mathbf{k} \mid V \rangle =(2\pi)^{N/2}(\Delta k)^{1/2}V_{\mathbf{k}}(\mathbf{p})$. For $\mathbf{k}=0$, the first term in the left-hand side of Eq. (2.20) vanishes and we obtain $\langle \mathbf{0} \mid H_1\rangle=\langle \mathbf{0} \mid V\rangle$, i.e., $H_1(\mathbf{p})=\Delta k\, V_0(\mathbf{p})$, this being called the secular term of the Hamiltonian. For $\mathbf{k}\neq\mathbf{0}$, we have

$$F_{\mathbf{k}1}(\mathbf{p})=\frac{iV_{\mathbf{k}}(\mathbf{p})}{\mathbf{k}\cdot\boldsymbol{\omega}} , \tag{2.21}$$

where $\mathbf{k}\cdot\boldsymbol{\omega}=k_1\omega_1+k_2\omega_2+\cdots+k_N\omega_N$ and $\omega_i=\partial H_0/\partial p_i$. Similarly we can solve the second equation in Eq. (2.13) and higher-order equations for $F_{\mathbf{k}n}(\mathbf{p})$ and $H_n(\mathbf{p})$, step by step, and obtain

$$H_2(\mathbf{p})=-\frac{\Delta k}{2}\sum_{\mathbf{k}}{}'\frac{\partial}{\partial \mathbf{p}}\cdot\mathbf{k}\frac{\Delta k \mid V_{\mathbf{k}}\mid^2}{\mathbf{k}\cdot\boldsymbol{\omega}} , \tag{2.22a}$$

$$F_{\mathbf{k}2}(\mathbf{p})=\frac{i}{\mathbf{k}\cdot\boldsymbol{\omega}}\sum_{\mathbf{k}'}{}'\left[-\frac{V_{\mathbf{k}-\mathbf{k}'}}{(\mathbf{k}-\mathbf{k}')\cdot\boldsymbol{\omega}}(\mathbf{k}-\mathbf{k}')\cdot\left[\frac{\partial(\Delta k\, V_{\mathbf{k}'})}{\partial \mathbf{p}}\right] + \left[\frac{\partial}{\partial \mathbf{p}}\cdot\mathbf{k}'\frac{V_{\mathbf{k}-\mathbf{k}'}}{(\mathbf{k}-\mathbf{k}')\cdot\boldsymbol{\omega}}\right]\Delta k\, V_{\mathbf{k}'}\right] , \tag{2.22b}$$

and so on. Note that there appear the so-called small denominators $(\mathbf{k}\cdot\boldsymbol{\omega})$ in the solutions. Thus, the above solutions are still formal and not well defined at this stage. In the next section we will show that if some of the Fourier spectrum is continuous, then the solutions become well defined by a suitable analytic continuation of $\mathbf{k}$ to the complex plane.

III. TRANSFORMATION OPERATOR WITH CONTINUOUS SPECTRUM

In order to make our argument transparent without using intricate notation, we hereafter restrict the number of degrees of freedom to $N=2$. Extension to arbitrary N is straightforward. For convenience in the following argument, we redefine the unperturbed Hamiltonian in Eq. (2.10) to include the secular term so that $gV_0=0$ holds in the new perturbation. We assume that the spectrum of k_2 is discrete in the domain of phase space in which we are interested, while k_1 has a continuous spectrum in the limit of $p_1\to p_{sx}$, where p_{sx} is a certain value of momentum in the domain. In Sec. IV we will show by specific examples that if there is a separatrix which comes from and goes to a hyperbolic fixed point in the phase space of the unperturbed system, then the spectrum becomes continuous in suitable canonical variables at the separatrix. In the limit of the continuous spectrum, i.e., $\Delta k_1\to 0$, the Fourier series with respect to k_1 reduces to a Fourier integral.

Let us consider the time evolution of the system. The evolution is governed by the Liouville equation

$$i\frac{\partial}{\partial t}\rho(\mathbf{q},\mathbf{p},t)=L_H\rho(\mathbf{q},\mathbf{p},t) . \tag{3.1}$$

Here ρ is the distribution function of the ensemble of the system in phase space, and L_H is called the Liouvillian, which is defined as a Lie derivative generated by the Hamiltonian. Corresponding to the decomposition of the Hamiltonian, the Liouvillian is decomposed into two parts, the unperturbed Liouvillian and the perturbation:

$$L_H=L_0+g\,\delta L , \tag{3.2}$$

where $L_0=L_{H_0}$ and $\delta L=L_V$. Because $L_0=-i\boldsymbol{\omega}\cdot\partial/\mathbf{q}$ is simply the derivative operator, it is clear that the complete orthonormal basis of the Fourier expansion Eq. (2.15) is just the eigenfunction of L_0 with the periodic boundary condition belonging to the eigenvalue $\mathbf{k}\cdot\boldsymbol{\omega}$. In the bra-ket notation, it is represented in terms of the projection operator by

$$L_0P_{\mathbf{k}}=(\mathbf{k}\cdot\boldsymbol{\omega})P_{\mathbf{k}} . \tag{3.3}$$

Our interest is in how the Liouville equation, Eq. (3.1) is transformed by the operator Λ_F defined in Eq. (2.8). To consider this problem, we introduce new notations $\tilde{\rho}=\Lambda_F^{-1}\rho$ and $\varphi=\Lambda_F^{-1}L_H\Lambda_F$. Then, we obtain from Eq. (3.1)

$$i\frac{\partial}{\partial t}\tilde{\rho}=\varphi\tilde{\rho} . \tag{3.4}$$

The evolution operator φ is called the "collision operator." We construct φ by using the perturbation expansion for F which is given in Eq. (2.10). To talk about the evolution, however, we must distinguish between two extremely different cases: one is the evolution of the trajectory and another is the evolution of the distribution function which has the δ-function singularity in the Fourier representation k_1 at the initial time $t=0$.

For the first case, i.e., the trajectory, the distribution function is given by

$$\rho(\mathbf{p},\mathbf{q},0)=\delta(\mathbf{q}-\mathbf{q}_0)\delta(\mathbf{p}-\mathbf{p}_0) =\frac{\Delta k}{(2\pi)^2}\sum_{\mathbf{k}}\delta(\mathbf{p}-\mathbf{p}_0)e^{i(\mathbf{q}-\mathbf{q}_0)\cdot\mathbf{k}} . \tag{3.5}$$

In this case the Fourier component with $k_1=0$ has the same order of magnitude as the component having $k_1\neq 0$. Therefore, in the limit of the continuous spectrum

$\Delta k_1 \rightarrow 0$, we can neglect the contribution from the component having $k_1=0$ to the integration of k_1.

For the second case, the distribution function is more precisely defined by the Fourier expansion

$$\rho(\mathbf{p},\mathbf{q},0)=\frac{\Delta k}{(2\pi)^2}\sum_{k_2}\left[\rho_{0,k_2}(\mathbf{p}) + \Delta k_1 \sum_{k_1}{}' \rho_{k_1,k_2}(\mathbf{p}) e^{ik_1 q_1}\right] e^{ik_2 q_2} . \tag{3.6}$$

Here ρ_{0,k_2} stands for the component having $k_1=0$ and ρ_{k_1,k_2} for the component having $k_1 \neq 0$. We assume that ρ_{0,k_2} and ρ_{k_1,k_2} have finite values in the limit of $\Delta k_1 \rightarrow 0$. That is, the distribution function has the $\delta(k_1)$ singularity in the Fourier integral of k_1. Note that the Fourier component having $k_1=0$ is $1/\Delta k_1$ times larger than the one having $k_1 \neq 0$. Therefore, ρ_{0,k_2} plays a distinctive role in this case, in contrast to the case of the trajectory. The importance of the existence of the δ-function singularity to obtain irreversible kinetic equations for systems with an infinite number of degrees of freedom was first pointed out by Prigogine and Balescu.[4] We will discuss the physical meaning of the δ-function singularity in more detail in Sec. V.

Let us first consider the case of the trajectory. In the lowest-order approximation of g the old momentum p_i^0 ($i=1,2$) is related to the new canonical variables $(\mathbf{q},\mathbf{p})$ by

$$p_i^0=\Lambda_{F_1}^{-1} p_i = p_i - g\, \Delta k \sum_{\mathbf{k}}{}' \frac{k_i V_{\mathbf{k}}}{\mathbf{k}\cdot\boldsymbol{\omega}} e^{i\mathbf{k}\cdot\mathbf{q}} . \tag{3.7}$$

Since the Hamiltonian is cyclic in the new representation, the solution of $p_i(t)$ and $q_i(t)$ is given in this approximation by $p_i(t)=\text{const}$ and $q_i(t)=\omega_i t + q_{0i}$. Substituting them in Eq. (3.7), we obtain the solution for $p_i^0(t)$. This solution is, however, still formal, because Eq. (3.7) includes the small denominator. Note that if we take the continuous limit $\Delta k_1 \rightarrow 0$, then the second term in the right-hand side reduces to the following type of the Cauchy integral which is evaluated on the real z axis,

$$\Phi(z)=\int_{-\infty}^{+\infty} dx \frac{f(x)}{x-z} . \tag{3.8}$$

As discussed in detail by Balescu,[6] if the function $f(x)$ satisfies suitable analytic conditions, which we assume to be satisfied in our case, then the Cauchy integral is well defined but has finite discontinuities on the real axis of z. This means that the solution of Eq. (3.7) is well defined in the continuous limit $\Delta k_1 \rightarrow 0$, but we need a physical boundary condition to determine the Riemann sheet of the analytic continuation of k_1 to evaluate the value of Eq. (3.7). To do it, we notice that the above argument has a close analogy with scattering theory in quantum mechanics when we distinguish between the incoming plane wave and the outgoing plane wave.[17] By analogy, we impose the boundary condition that the perturbed solution $p_1^0(t)$ in Eq. (3.7) reduces to the unperturbed solution p_1 in the limit of $t \rightarrow -\infty$. Then, we obtain the solution

$$p_{1+}^0(t)=p_i - g\, \Delta k_2 \sum_{k_2} \int_{-\infty}^{+\infty} dk_1 \frac{k_1 V_{\mathbf{k}}(\mathbf{p})}{\mathbf{k}\cdot\boldsymbol{\omega} - i\varepsilon} e^{i\mathbf{k}\cdot(\boldsymbol{\omega}t+\mathbf{q}_{01})} , \tag{3.9}$$

where ε is a positive infinitesimal. The corresponding generating function is given by

$$F_{1+}(\mathbf{q},\mathbf{p})=\Delta k_2 \sum_{k_2} \int_{-\infty}^{+\infty} dk_1 \frac{iV_{\mathbf{k}}(\mathbf{p})}{\mathbf{k}\cdot\boldsymbol{\omega}-i\varepsilon} e^{i\mathbf{k}\cdot\mathbf{q}} . \tag{3.10}$$

In Sec. IV we will apply the above boundary condition to specific nonlinear systems with a hyperbolic fixed point. Then we will show that Eq. (3.9) is the solution on the unstable manifold. Similarly, if we impose the boundary condition such that $p_1^0(t) \rightarrow p_1$ in the limit $t \rightarrow +\infty$, then we obtain the solution $p_{1-}^0(t)$ on the stable manifold and the generating function $F_{1-}(\mathbf{q},\mathbf{p})$ which has the same form as p_{1+}^0 and F_{1+} except that ε is replaced by $-\varepsilon$.

Next we consider the case of the distribution function Eq. (3.6) which has the δ-function singularity. We first consider the time evolution of the component $\tilde{\rho}_{0,k_2}$. Because the Hamiltonian is cyclic in the new representation, the evolution operator φ is commutable with the projection operator $P_{\mathbf{k}}$. This implies that $\tilde{\rho}_{0,k_2}$ obeys the closed equation

$$i\frac{\partial}{\partial t}\langle 0,k_2 | \tilde{\rho}(t)\rangle = \langle 0,k_2 | \Lambda_F^{-1} L_H \Lambda_F | 0,k_2\rangle \langle 0,k_2 | \tilde{\rho}(t)\rangle . \tag{3.11}$$

The matrix element in Eq. (3.11) is given in the lowest-order approximation by

$$\begin{aligned}\langle 0,k_2 | \Lambda_F^{-1} L_H \Lambda_F | 0,k_2\rangle &\simeq g^2 \langle 0,k_2 | \varphi_2 | 0,k_2 \rangle \\ &= g^2 \langle 0,k_2 | [(-iL_1)\delta L + L_1 L_0 L_1 \\ &\quad + \delta L(+iL_1)] | 0,k_2\rangle ,\end{aligned} \tag{3.12}$$

where

$$\begin{aligned}\langle 0,k_2 | (-iL_1)\delta L \; | 0,k_2\rangle = \sqrt{\Delta k} \sum_{\mathbf{k}'} &\left[-\frac{\partial}{\partial \mathbf{p}}\cdot(\mathbf{k}_2-\mathbf{k}')\frac{V_{\mathbf{k}_2-\mathbf{k}'}}{(\mathbf{k}_2-\mathbf{k}')\cdot\boldsymbol{\omega}} + \left[\frac{\partial}{\partial p_2}\frac{k_2 V_{\mathbf{k}_2-\mathbf{k}'}}{(\mathbf{k}_2-\mathbf{k}')\cdot\boldsymbol{\omega}}\right]\right]\Delta k \\ &\times\left[-V_{\mathbf{k}'-\mathbf{k}_2}(\mathbf{k}'-\mathbf{k}_2)\cdot\frac{\partial}{\partial \mathbf{p}} + \left[\frac{\partial}{\partial p_2} k_2 V_{\mathbf{k}'-\mathbf{k}_2}\right]\right]\sqrt{\Delta k} ,\end{aligned} \tag{3.13}$$

and so on, where we have used the notation $\mathbf{k}_2$ for the vector $(0,k_2)$.

For sufficiently small Δk_1, we can replace the summation of k_1 by the integration, and we obtain the Cauchy integral once again. In order to determine the branch of analytic continuation, we impose the physical boundary condition that the distribution function $\tilde{\rho}_{0,k_2}$ approaches the steady solution in the limit of $t \to +\infty$. In other words, we impose the condition that the Hermitian part of the collision operator $\langle \mathbf{k}_2 | i\varphi_2 | \mathbf{k}_2 \rangle$ is non-negative in the Hilbert space defined by phase functions with the periodic boundary condition for $\mathbf{q}$. For a given analytic continuation, this condition is tested in a way similar to the proof of the H theorem in the kinetic equation of an infinitely large system.[7] Then we see that this condition uniquely determines the analytic continuation of the matrix element of Λ_F which is put between the states $|\mathbf{k}_2\rangle$ and $|\mathbf{k}'\rangle$ in the lowest-order approximation

$$\langle \mathbf{k}_2 | \Lambda_F | \mathbf{k}' \rangle \simeq ig \langle \mathbf{k}_2 | L_{1-} | \mathbf{k}' \rangle , \tag{3.14a}$$

$$\langle \mathbf{k}' | \Lambda_F | \mathbf{k}_2 \rangle \simeq ig \langle \mathbf{k}' | L_{1+} | \mathbf{k}_2 \rangle . \tag{3.14b}$$

Here $L_{1\pm}$ is the Lie derivatives generated by $F_{1\pm}(\mathbf{p},\mathbf{q})$ which have been defined in Eq. (3.10) and following.

To complete the form of the operator Λ_F, we must also determine the analytic continuation of the matrix element $\langle \mathbf{k} | \Lambda_F | \mathbf{k}' \rangle$ for $k_1 \neq 0$ and $k_1' \neq 0$. For this element, we impose the boundary condition that if the collision operator $\langle \mathbf{k} | \varphi_2 | \mathbf{k} \rangle$ operates on the distribution function of the trajectory corresponding to Eq. (3.5), then it gives an evolution on the unstable manifold. Notice that for the case of the trajectory, the matrix element Eq. (3.12) is irrelevant. Then we obtain from Eq. (3.10) that

$$\langle \mathbf{k} | \Lambda_F | \mathbf{k}' \rangle = ig \langle \mathbf{k} | L_{1+} | \mathbf{k}' \rangle . \tag{3.14c}$$

An interesting observation of the results Eqs. (3.14) is that the generating function of the transformation operator Λ_F does not reduce to a single function F_{1+} because of Eq. (3.14a). Owing to this fact, Λ_F is not a unitary operator, but a star-unitary operator, i.e.,

$$\Lambda_F^{\dagger}(L_H) = \Lambda_F^{-1}(-L_H) , \tag{3.15}$$

where $\Lambda_F^{\dagger}$ stands for the Hermitian conjugate of Λ_F. The concept of the star-unitarity operator was introduced by Prigogine *et al.*[9] to discuss the origin of irreversibility for infinitely large conservative systems. The nonunitarity is essential to discuss irreversible evolution for the distribution function which has the δ-function singularity. Note, however, that if the transformation operator Λ_F acts on the distribution function of the trajectory, then we can neglect the contribution from the matrix elements in Eqs. (3.14a) and (3.14b), so that we cannot distinguish the above operator Λ_F from the unitary operator Λ_{F_+} which consists of a single generating function F_+. This implies that if we observe time evolution of the trajectory, then we cannot see any irreversibility, while if we observe time evolution of the ensemble with the δ-function singularity, then we can see it in the same system. In this sense, we have a compatibility of the irreversibility with the reversibility in the nonlinear Hamiltonian system.

From the transformation operator Eqs. (3.14) we can explicitly construct the kinetic equation. For example, the momentum distribution function which is just $\tilde{\rho}_{0,0}(\mathbf{p})$ in Eq. (3.6) is governed by the diffusion equation for sufficiently small Δk_1,

$$\frac{\partial}{\partial t}\tilde{\rho}_{0,0}(\mathbf{p},t) = \pi g^2 \sum_{\mathbf{k}} \frac{\partial}{\partial \mathbf{p}} \cdot \mathbf{k}\,\Delta k\, | V_{\mathbf{k}} |^2 \delta(\mathbf{k}\cdot\boldsymbol{\omega})\mathbf{k}\cdot\frac{\partial}{\partial \mathbf{p}} \Delta k \tilde{\rho}_{0,0}(\mathbf{p},t) . \tag{3.16}$$

Here we have used the Plomelj formula

$$\lim_{\varepsilon\to 0+} \frac{1}{x \mp i\varepsilon} = \mathrm{P}\frac{1}{x} \pm i\pi\delta(x) , \tag{3.17}$$

where P stands for the principal part thereof. Equation (3.16) completely coincides with the equation for describing Chirikov's diffusion process in the stochastic layer around the unperturbed separatrix,[1] which has been obtained based upon the different philosophy that we have collected the most diverging terms in time in the limit of $t \to \infty$ and $g \to 0$. Note that the right-hand side of Eq. (3.16) is proportional to a small factor Δk. Hence, the right-hand side has a contribution only for sufficiently large time t, such as the effect of the cross section in the scattering problem.[5,7]

IV. EXAMPLES OF THE SYSTEM

In this section we give two examples which reduce the Hamiltonian Eq. (2.9) with continuous spectrum in certain canonical variables. The first example is a system with a double-well potential and the second is a nonlinear pendulum. Both are coupled with a linear spring.

For the first example, the Hamiltonian is given by

$$H(\mathbf{x},\mathbf{y};g) = H_0(\mathbf{x},\mathbf{y}) + gV(\mathbf{x}) , \tag{4.1}$$

where $H_0 = H_1 + H_2$ with

$$H_1 = \frac{y_1^2}{2} - \frac{x_1^2}{2} + \frac{x_1^4}{4}, \quad H_2 = \omega_2 y_2 , \tag{4.2}$$

and

$$gV = -\tfrac{1}{2} g x_1^2 \cos x_2 , \tag{4.3}$$

and y_i is a generalized momentum which is a canonical conjugate to x_i. The unperturbed system with H_1 has a hyperbolic fixed point at the origin and two elliptic fixed points at $(\pm 1, 0)$ in the phase space of (x_1, y_1). The energy on the separatrix is $H_1 = 0$.

In order to reduce the Hamiltonian equation (4.1) to the form of Eq. (2.9) we introduce new canonical variables (q_1, p_1) in which the Hamiltonian H_1 becomes cyclic in the form

$$H_1 = \tfrac{1}{4}(p_1^2 - 1) . \tag{4.4}$$

The new variables are given by the following canonical transformations.

(i) For $0 \le p_1 < 1$,

$$x_1 = \pm\sqrt{1+p_1}\,\mathrm{dn}\left[\frac{\sqrt{2(1+p_1)}}{p_1}q_1, c\right],$$
$$y_1 = \mp\frac{2p_1}{\sqrt{1+p_1}}\mathrm{sn}\left[\frac{\sqrt{2(1+p_1)}}{p_1}q_1, c\right] \times \mathrm{cn}\left[\frac{\sqrt{2(1+p_1)}}{p_1}q_1, c\right]. \tag{4.5a}$$

(ii) For $p_1 = 1$ (at the separatrix),

$$x_1 = \pm\sqrt{2}\,\mathrm{sech}(2q_1),$$
$$y_1 = \mp\sqrt{2}\tanh(2q_1)\mathrm{sech}(2q_1). \tag{4.5b}$$

(iii) For $p_1 > 1$,

$$x_1 = \sqrt{1+p_1}\,\mathrm{cn}\left[\frac{2q_1}{\sqrt{p_1}}, \frac{1}{c}\right],$$
$$y_1 = -\sqrt{p_1(1+p_1)}\,\mathrm{sn}\left[\frac{2q_1}{\sqrt{p_1}}, \frac{1}{c}\right]\mathrm{dn}\left[\frac{2q_1}{\sqrt{p_1}}, \frac{1}{c}\right], \tag{4.5c}$$

where c in Eq. (4.5a) and c^{-1} in Eq. (4.5c) are the squares of the moduli of the Jacobi elliptic functions[18] defined by

$$c = \frac{2p_1}{1+p_1}. \tag{4.6}$$

The signs in Eqs. (4.5a) and (4.5b) correspond to the branches of the motion. Note that our canonical transformations are well defined and continuous at the separatrix $H_1 = 0$.

Applying the canonical transformation in Eq. (4.5) to the Hamiltonian in Eq. (4.1) and putting $q_2 = x_2$, $p_2 = y_2$, we obtain the new Hamiltonian

$$H = \tfrac{1}{4}(p_1^2 - 1) + \omega_2 p_2 + g v(q_1, p_1)\cos q_2, \tag{4.7}$$

where

$$v(q_1,p_1) = \begin{cases} -\tfrac{1}{2}\mathrm{dn}^2\left[2q_1\frac{\sqrt{2-c}}{c}, c\right], & 0 \le p_1 \le 1 \\ -\tfrac{1}{2}\mathrm{cn}^2\left[2q_1\left[\frac{2-c}{c}\right]^{1/2}, \frac{1}{c}\right], & p_1 > 1. \end{cases} \tag{4.8}$$

The Fourier component of the interaction is given by

$$V_{k_1,k_2} = \begin{cases} -\frac{c}{8\sqrt{2-c}}\left[\frac{E}{p}\delta_{k_1,0} + \frac{c}{4\sqrt{2-c}}\frac{k_1}{\sinh(k_1K'c/2\sqrt{2-c})}(1-\delta_{k_1,0})\right](\delta_{k_2,1}+\delta_{k_2,-1}), & 0 \le p_1 \le 1 \\ -\frac{c}{8\sqrt{2-c}}\left[\frac{\sqrt{c}}{p}\left[E_- + \frac{c'}{c}K_-\right]\delta_{k_1,0} + \frac{c}{4\sqrt{2-c}}\frac{k_1}{\sinh(k_1K'_-\sqrt{c}/2\sqrt{2-c})}(1-\delta_{k_1,0})\right] & \\ \times(\delta_{k_2,1}+\delta_{k_2,-1}), & p_1 > 1. \end{cases} \tag{4.9}$$

Here $k_1 = n\,\Delta k_1$ with any integer n and

$$\Delta k_1 = \begin{cases} \frac{2\pi\sqrt{2-c}}{Kc}, & 0 < p_1 \le 1 \\ \frac{2\pi}{K_-}\left[\frac{2-c}{c}\right]^{1/2}, & p_1 > 1 \end{cases} \tag{4.10}$$

and $K \equiv K(c)$, $E \equiv E(c)$ are complete elliptic integrals of first and second kind with the square of the modulus c, respectively. K' is the complementary complete elliptic integral defined by $K' \equiv K(c')$ with $c' = 1 - c$, and $K_- \equiv K(c^{-1})$, $E_- \equiv E(c^{-1})$, and so on.

The second example is a coupled nonlinear pendulum with a linear spring, the Hamiltonian of which is given by

$$H(\mathbf{x},\mathbf{y};g) = H_0(\mathbf{x},\mathbf{y}) + gV(\mathbf{x}), \tag{4.11}$$

where $H_0 = H_1 + H_2$ with

$$H_1 = y_1^2 + \tfrac{1}{2}(1-\cos x_1), \quad H_2 = \omega_2 y_2 \tag{4.12}$$

and

$$gV = \frac{g}{2}\cos x_1 \cos x_2. \tag{4.13}$$

The unperturbed pendulum H_1 has a hyperbolic fixed point at $(\pi, 0)$ and the elliptic fixed point at the origin of phase space (x_1, y_1). The energy on the separatrix is $H_1 = 1$. The canonical transformations are given by the following.

(i) For $p_1 > 1$ (rotation),

$$\sin\frac{x_1}{2} = \pm\mathrm{sn}\left[\frac{q_1}{2}, c\right], \quad y_1 = \pm\mathrm{dn}\left[\frac{q_1}{2}, c\right]. \tag{4.14a}$$

(ii) For $p_1 = 1$ (at the separatrix),

$$\sin\frac{x_1}{2} = \pm\tanh\frac{q_1}{2}, \quad y_1 = \pm\mathrm{sech}\frac{q_1}{2}. \tag{4.14b}$$

(iii) For $0 \le p_1 < 1$ (libration),

$$\sin\frac{x_1}{2} = p_1\mathrm{sn}\left[\frac{\sqrt{c}}{2}q_1, \frac{1}{c}\right], \quad y_1 = p_1\mathrm{cn}\left[\frac{\sqrt{c}}{2}q_1, \frac{1}{c}\right], \tag{4.14c}$$

where $c=1/p_1^2$. By putting $q_2=x_2$, $p_2=y_2$, the Hamiltonian Eq. (4.11) becomes

$$H=p_1^2+\omega_2 p_2+gv(q_1,p_1)\cos q_2 \ , \tag{4.15}$$

where

$$v(q_1,p_1)=\begin{cases} \frac{1}{2}-\mathrm{sn}^2\left[\frac{q_1}{2},c\right], & p_1\ge 1 \\ p_1^2\left[\frac{1}{2}-\mathrm{sn}^2\left[\frac{\sqrt{c}}{2}q_1,\frac{1}{c}\right]\right], & 0<p_1<1 \ . \end{cases} \tag{4.16}$$

The Fourier component of the interaction is given by

$$V_{k_1,k_2}=\begin{cases} 2p_1^2\left\{\frac{1}{\pi}\left[E+\left[\frac{c}{2}-1\right]K\right]\delta_{k_1,0}+\frac{k_1}{\sinh(2k_1K')}(1-\delta_{k_1,0})\right\}(\delta_{k_2,1}+\delta_{k_2,-1}), & p_1\ge 1 \\ 2p_1^2\left\{\frac{1}{\pi}\left[\sqrt{c}E_-+\left[\frac{1}{2}-c\right]K_-\right]\delta_{k_1,0}+\frac{k_1}{\sinh(2p_1k_1K'_-)}(1-\delta_{k_1,0})\right\}(\delta_{k_2,1}+\delta_{k_2,-1}), & 0<p_1<1 \end{cases} \tag{4.17}$$

where $k_1=n\,\Delta k_1$ with integer n and

$$\Delta k_1=\begin{cases} \frac{\pi}{2K}, & p_1\ge 1 \\ \frac{\sqrt{c}\pi}{2K_-}, & 0<p_1<1 \ . \end{cases} \tag{4.18}$$

Note that in the limit of the separatrix, i.e., $p_1\to 1$, the Fourier spectrum of k_1 becomes continuous, i.e., $\Delta k_1\to 0$, for both cases of the example.

Let us now show that the solution given by Eq. (3.9) corresponds in these examples to the trajectory on the unstable manifold. We first note that the generating function F_{1+} in Eq. (3.10) vanishes in the limit of $t\to-\infty$. Hence, in this asymptotic limit, we have $p_{1+}^0\to p_1=1$ and $q_{1+}^0\to\omega_1(t-t_0)$ where t_0 is a constant. Substituting these limiting values in the canonical transformations of Eqs. (4.5b) and (4.14b), we see that the solutions approach their hyperbolic fixed point in (x_1,y_1) space in the limit of $t\to-\infty$. This implies that the solution Eq. (3.9) is just the solution on the unstable manifold. Similarly, we can prove that the solution p_{1-}^0 and q_{1-}^0 generated by F_{1-} corresponds to the trajectory on the stable manifold.

V. MEANING OF THE δ-FUNCTION SINGULARITY

In Sec. III we showed that the δ-function singularity is essential for the irreversible kinetic equation Eq. (3.10) to have a meaning in nonlinear systems which have a hyperbolic fixed point in phase space. In this section, we discuss the physical meaning of the δ-function singularity in more detail.

Our assertion is the following: If the initial distribution function includes a homoclinic point with a finite measure, such as the step function, then the distribution function has the δ-function singularity no matter how small the measure is. Here the homoclinic point is defined as a point of transverse intersection of the stable and unstable manifolds in a Poincaré surface of section.

To make our assertion clear, let us consider the example of the nonlinear pendulum given in Eq. (4.7). The system is periodic in x_1, so that we restrict the domain of x_1 to $-\pi\le x_1\le\pi$. Then, the hyperbolic fixed point corresponds to $x_1=\pm\pi$. By the canonical transformation Eq. (4.14) the hyperbolic fixed point is mapped to $q_1=\pm 2K(c)$ for $c\le 1$. We first consider a special initial distribution function which includes the hyperbolic fixed point and is given by

$$\rho(\mathbf{x},\mathbf{y})=C\delta[y_1^2+\tfrac{1}{2}(1-\cos x_1)-p_{10}^2]\delta(y_2-p_{20}) \times[\Theta(x_1-x_a)+\Theta(x_b-x_1)] \ , \tag{5.1}$$

where p_{10}, p_{20}, x_a, and x_b ($<x_a$) are given constants, C is a normalization constant which depends on x_a and x_b, and $\Theta(x)$ is the step function defined by

$$\Theta(x)=\begin{cases} 1, & x\ge 0 \\ 0, & x<0 \ . \end{cases} \tag{5.2}$$

In other words, the ensemble is restricted to the unperturbed energy surface, and the angle x_1 is distributed as the step function around the hyperbolic fixed point. Because the effect of the perturbation is small around the hyperbolic fixed point, we prepare the initial distribution Eq. (5.1) near the hyperbolic point, i.e., $x_a\simeq\pi$ and $x_b\simeq-\pi$. In the new representation $(\mathbf{q},\mathbf{p})$, the distribution function Eq. (5.1) is written as

$$\rho(\mathbf{q},\mathbf{p})=C\delta(p_1^2-p_{10}^2)\delta(p_2-p_{20}) \times[\Theta(q_1-q_a)+\Theta(q_b-q_1)] \ , \tag{5.3}$$

where q_i ($i=a,b$) is given as the solution of Eq. (4.14) with $x_1=x_i (i=a,b)$ and $c=1/p_{10}^2$. In the continuous-spectrum limit, i.e., $p_{10}\to 1$, the domain of q_1 becomes $-\infty\le q_1\le+\infty$. Thus, we can represent the step function in Eq. (5.3) by the Fourier integral, and obtain

$$\rho(\mathbf{q},\mathbf{p})=C\delta(p_1^2-1)\delta(p_2-p_{20}) \times\frac{1}{2\pi i}\int_{-\infty}^{+\infty}dk_1\left[\frac{1}{k_1-i\varepsilon}e^{ik_1(q_1-q_a)}-\frac{1}{k_1+i\varepsilon}e^{ik_1(q_1-q_b)}\right] , \tag{5.4}$$

where ε is a positive infinitesimal. By applying the

Plomelj formula Eq. (3.17), we can conclude that the distribution function Eq. (5.4) has the δ-function singularity in the Fourier representation. An important observation of this example is that if the distribution function includes the hyperbolic fixed point with a finite width in x_1 space, then it has the δ-function singularity no matter how small the width.

Let us now consider a more general distribution function with a finite measure which does not necessarily include the hyperbolic fixed point, but includes at least one homoclinic point. This means that the ensemble contains continuously distributed points on the unstable manifold on both sides of the stable manifold. By the definition of the homoclinic point, it approaches the hyperbolic fixed point in the limit of $t \to +\infty$. Therefore, because the unstable manifold intersects transversely with the stable manifold at the homoclinic point, the ensemble will eventually distribute around the hyperbolic fixed point with a finite width, no matter how small the initial width. Consequently, the distribution function has the δ-function singularity as we have asserted. Because infinitely many homoclinic points are distributed in a very complicated fashion around the hyperbolic fixed point (indeed they are distributed as a Cantor set[15]), it seems to us almost impossible to construct a distribution function which does not have the δ-function singularity, except for a preparation with infinite accuracy such as the distribution function for a single trajectory given in Eq. (3.5).[20]

VI. DISCUSSION: IRREVERSIBILITY AND NONINTEGRABILITY

In the preceding section we have shown that the irreversible kinetic equation (3.16) has meaning when the system has a homoclinic point. On the other hand, one can prove by constructing Smale's horseshoe map[19] around the homoclinic point that if the Hamiltonian system has a homoclinic point, then the system is nonintegrable.[14,15] In the following argument, we discuss this relation in more detail.

In the context of derivation of irreversible kinetic equations for infinitely large systems in nonequilibrium statistical mechanics, Prigogine[5] has summarized a dynamical condition for irreversibility as the "dissipativity condition." This condition states that if the collision operator is not identically zero, then the system has irreversibility. In the following argument we will show that the dissipativity condition is equivalent to the condition of the existence of the homoclinic point in nonlinear systems with two degrees of freedom which are coupled with a linear system such as the examples in Sec. IV. In this sense, Prigogine's dissipativity condition is equivalent to the nonintegrability condition.

In the nonlinear system coupled with a linear system, the criterion of the existence of the homoclinic point in the Poincaré surface of the section in (x_1, y_1) space is given by the Melnikov function[15,16] $\Delta(t,t_0)$ defined by

$$\Delta(t,t_0)=\Delta^+(t,t_0)-\Delta^-(t,t_0)\ , \tag{6.1}$$

where

$$\Delta^{\pm}(t,t_0)=\dot{x}_{1sx}(t-t_0)y_{1\pm}(t,t_0) -\dot{y}_{1sx}(t-t_0)x_{1\pm}(t,t_0)\ . \tag{6.2}$$

Here (x_{1sx}, y_{1sx}) is the unperturbed solution on the separatrix and $(x_{1\pm}, y_{1\pm})$ are the perturbed solutions on the unstable manifold $(+)$ and the stable manifold $(-)$, respectively, which satisfies the condition

$$\dot{x}_{1sx}(0)[x_{1\pm}(t_0,t_0)-x_{1sx}(0)] +\dot{y}_{1sx}(0)[y_{1\pm}(t_0,t_0)-y_{1sx}(0)]=0\ . \tag{6.3}$$

From Eqs. (6.1)—(6.3), we can easily obtain that

$$|\Delta(t_0,t_0)|=\{[\dot{x}_{1sx}(0)^2+[\dot{y}_{1sx}(0)]^2\}^{1/2} \times\{[x_{1+}(t_0,t_0)-x_{1-}(t_0,t_0)]^2 +[y_{1+}(t_0,t_0)-y_{1-}(t_0,t_0)]^2\}^{1/2}\ . \tag{6.4}$$

Therefore, the Melnikov function characterizes the distance between the unstable manifold and the stable manifold. If the Melnikov function $\Delta(t_0,t_0)$ is not identically zero but oscillates around zero as a function of t_0, then the unstable manifold intersects transversely with the stable manifold. Applying the perturbation expansion in Eq. (6.2) such that $\Delta_\pm=\Delta_0+g\Delta_{1\pm}+g^2\Delta_{2\pm}+\cdots$ around the unperturbed solution on the separatrix, we obtain after a simple manipulation that

$$g\dot{\Delta}_{1\pm}(t,t_0)=\{H_0,H\}_{sx}\ , \tag{6.5}$$

where $\{\ ,\ \}_{sx}$ stands for the Poisson bracket which is evaluated along the unperturbed solution on the separatrix. Note that the right-hand side of Eq. (6.5) does not depend on the representation, so we can calculate it in the new representation (q_1,p_1) that makes the unperturbed Hamiltonian cyclic. Then we obtain by the integration in time with suitable boundary conditions that

$$\Delta(t,t_0)\simeq\omega_1[p^0_{1+}(t,t_0)-p^0_{1-}(t,t_0)] =-2\pi i g\omega_1\Delta k\sum_{\mathbf{k}}k_1V_{\mathbf{k}}\delta(\mathbf{k}\cdot\boldsymbol{\omega})e^{i\mathbf{k}\cdot\mathbf{q}_0}\ , \tag{6.6}$$

where $q_{01}\equiv-\omega t_0$, and we have used the perturbed solutions with the summation sign which are given in Eq. (3.9) and following. Note that the right-hand side of Eq. (6.6) is independent of t in this approximation, so that it is equal to $\Delta(t_0,t_0)$. To see clearly the relation of the result Eq. (6.6) to the collision operator, we change the variable $\mathbf{p}$ in Eq. (3.16) such that $r_1=p_1$ and $r_2=H_0(p_1,p_2)$. Then, we obtain for the collision operator that

$$\pi g^2\sum_{\mathbf{k}}\frac{\partial}{\partial\mathbf{p}}\cdot\mathbf{k}\,\Delta k\ |V_{\mathbf{k}}|^2\delta(\mathbf{k}\cdot\boldsymbol{\omega})\mathbf{k}\cdot\frac{\partial}{\partial\mathbf{p}}\Delta k =\pi g^2\frac{\partial}{\partial r_1}\Delta k\sum_{\mathbf{k}}|k_1V_{\mathbf{k}}|^2\delta(\mathbf{k}\cdot\boldsymbol{\omega})\frac{\partial}{\partial r_1}\Delta k\ . \tag{6.7}$$

Comparing this result with Eq. (6.6), it is clear that if and only if the coefficient of Δk in the collision operator is not identically zero, then the Melnikov function is not identically zero. In this sense, the dissipativity condition is equivalent to the condition of the existence of the homoclinic point, i.e., the condition of the nonintegrability.

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[1]T. Y. Petrosky, Phys. Rev. A **29**, 2078 (1984).
[2]B. V. Chirikov, Phys. Rep. **52**, 263 (1979).
[3]L. Van Hove, Physica **21**, 517 (1955); **23**, 441 (1957).
[4]I. Prigogine and R. Balescu, Physica **25**, 281 (1959); **25**, 302 (1959); **26**, 145 (1960).
[5]I. Prigogine, *Non-Equilibrium Statistical Mechanics* (Interscience, New York, 1962).
[6]R. Balescu, *Statistical Mechanics of Charged Particles* (Interscience, New York, 1963).
[7]P. Résibois, in *Physics of Many-Particle Systems,* edited by E. Meeron (Gordon and Breach, New York, 1966).
[8]I. Prigogine, Cl. George, and F. Henin, Physica **45**, 418 (1969).
[9]I. Prigogine, Cl. George, F. Henin, and L. Rosenfeld, Chem. Scr. **4**, 5 (1973).
[10]Cl. George, Bull. Acad. R. Belg. Cl. Sci. **56**, 505 (1970).
[11]A. Deprit, Celestial Mechanics **1**, 12 (1969).
[12]R. L. Dewar, J. Phys. A **9**, 2043 (1976).
[13]J. R. Cary, Phys. Rep. **79**, 129 (1981).
[14]J. Moser, *Stable and Random Motions in Dynamical Systems* (Princeton University Press, Princeton, N.J., 1973).
[15]J. Guckenheimer and P. Holmes, *Nonlinear Oscillations, Dynamical Systems and Bifurcations of Vector Fields* (Springer, New York, 1983).
[16]V. K. Melnikov, Trans. Moscow Math. Soc. **12**, 1 (1963).
[17]M. Goldberger and R. Watson, *Collision Theory* (Wiley, New York, 1964).
[18]E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis,* 4th ed. (Cambridge University Press, Cambridge, England, 1980).
[19]S. Smale, *The Mathematics of Time* (Springer, New York, 1980).
[20]In other words, we need an infinite amount of information (i.e., negative entropy) to avoid the irreversible phenomena around the hyperbolic point.