Resonance overlap, secular effects, and nonintegrability: An approach from ensemble theory

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The time evolution of a classical multiresonance nonintegrable Hamiltonian system with few degrees of freedom is analyzed on the ensemble level. Time-dependent perturbation analysis is applied to the Liouville equation to determine the most secular series for the time evolution of the expectation value of some physical observables. In contrast to the so-called $\lambda^2 t$ expansion for thermodynamic systems, which is well known in nonequilibrium statistical physics, we find a $\sqrt{\lambda}t$ expansion in small nonintegrable systems with few degrees of freedom. This asymptotic expansion exists only on the level of ensemble but not on the level of trajectories. Moreover, the time symmetry of this expansion is broken as in nonequilibrium statistical mechanics. The relation of the Chirikov overlapping criterion to our approach is discussed.

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I. INTRODUCTION

Beginning in the 1950s Van Hove [1,2] (in quantum mechanics), and Prigogine and Balescu [3-7] (in classical mechanics) applied asymptotic perturbation analysis to the Liouville equation of Poincaré nonintegrable systems with infinite degrees of freedom [the so-called large Poincaré systems (LPS) [5,8–10]]. By collecting the most diverging terms in t (the most secular effect) arising from the resonance effects in the asymptotic limit (the so-called Van Hove's $\lambda^2 t$ limit with $t \rightarrow \infty$, $\lambda \rightarrow 0$, and keeping $\lambda^2 t$ finite, where λ is the coupling constant), they derived kinetic equations that break time symmetry. This important discovery revealed a deeper relation between the origin of irreversibility in the basic laws of physics and nonintegrability of dynamical systems due to the resonance singularities on the level of ensemble. This has then led to several important developments in modern nonequilibrium statistical physics, such as correlation dynamics [5], subdynamics and nonunitary transformations [9-16], the complex spectral representations of the Hamiltonian [17-20], and of the Liouville-von Neumann operator outside the Hilbert space [9,10,14,15,21].

Therefore, it is natural to ask if there is a similar asymptotic perturbation analysis for small classical nonintegrable Hamiltonian systems with few degrees of freedom. We will call these Hamiltonian systems "small Poincaré systems (SPS)" to emphasize their difference from systems with infinite degrees of freedom. We note that a major difference between LPS and SPS is that the spectrum of the unperturbed Liouville operator is continuous in LPS, while it is discrete in SPS.

It is well known that nonintegrability leads to the failure of ordinary perturbation analysis due to resonance singularities appearing in the series expansion (the small denominator problem with a division by zero) [22,23]. In LPS with continuous spectrum, there is a well-defined mathematical meaning of the division by zero as an appearance of distributions (generalized functions) [5], such as Dirac's δ function in the continuous variables at the resonance points. The resonance singularities then lead to secular effects that are characterized by the $\lambda^2 t$ expansion. However, one cannot apply this manipulation directly to SPS since there are no such distributions for the discrete spectrum. Nevertheless, one possible extension has been achieved by one of the authors (T.P.) in SPS by restricting one's interest to a domain of phase space, such as inside the stochastic layer around separatrices, in which the characteristic period is so long that one can approximate the discrete spectrum by a continuous one [24–26]. In this case, one can derive a kinetic equation that has essentially the same structure as the one in LPS (see also Ref. [22] for a similar discussion of this consideration). This kinetic equation describes irreversible processes in SPS, such as the Arnold diffusion inside a stochastic layer.

In this paper, we will deal with a more challenging problem of extending the asymptotic perturbation analysis to SPS for situations where the characteristic periods are not so long, such as the case outside the stochastic layer. In this case, one can no longer approximate the discrete spectrum by a continuous one. A way out of the difficulty due to the discrete spectrum, as will be shown, is to deal with an ensemble dynamics governed by the Liouville equation instead of a trajectory dynamics governed by the Hamilton's equation of motion. We will consider the ensemble average of observables so that the small denominators appearing in the perturbation series can be treated as a distribution of the continuous generalized momenta under the phase space integration.

The need to consider the small denominator under the phase space integration for SPS was recognized some years ago by Prigogine, Grecos, and George [27]. By simply applying the kinetic theory developed for LPS in nonequilibrium statistical mechanics they have suggested that the same kinetic description might exist in SPS. However, this idea, while going in the right direction, is not enough to solve the small denominator problem for the discrete spectrum case in SPS. In this paper, we will show some differences in dealing with the small denominator problem in SPS from LPS.

Let us assume that the Liouville operator L of the system consists of the unperturbed integrable part L_0 and the inter-

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action part δL that makes the whole system nonintegrable. In the case of LPS, one may perform the integration over the continuous spectrum of L_0 in each small denominator (propagator) which is understood as an individual distribution in the continuous wave vectors. Hence, after the integrations over the wave vectors for each propagator, a product of two propagators with two independent continuous wave vectors gives us a product of two ordinary functions.

On the other hand, in the case of SPS, the small denominator is treated as a distribution in the momenta (instead of the wave vectors) under the phase space integration of the ensemble average as mentioned above. As a result, a product of two propagators should be treated as a *single distribution* in the momenta, but not as a product of two distributions. We will show that the product of two propagators may lead to extra singularities of the resonances, which does not appear if we perform the integration over the continuous spectrum on each propagator as in the case of LPS. These new singularities then lead to stronger secular effects in SPS than in LPS.

We note that the above treatment of the small denominator is possible only on the ensemble level but not on the level of trajectory. In other words, we are extracting some information of the dynamics which appears only on the ensemble level. One of the unique properties of the ensemble approach is the appearance of broken time symmetry.

The main results of this paper are as follows: (1) By considering the evolution of the expectation value of observables we find that the most secular effect from each single resonance is given by an asymptotic series with time dependence $\lambda^{3/2}(\sqrt{\lambda}t)^{4m-3}$ for $m \ge 1$ in comparison to the $(\lambda^2 t)^m$ contribution for LPS. (2) We consider the contributions from the interference between resonances and find secular effects with oscillation corresponding to the higher harmonics of the system.

In order to carry out our procedure more clearly we will apply the asymptotic perturbation analysis to a nonintegrable multiresonance Hamiltonian system with two degrees of freedom

$$H(J_1, J_2, \theta_1, \theta_2) = H_0(J_1, J_2) + \lambda_1 V_1(\theta_1) + \lambda_2 V_2(\theta_1, \theta_2),$$
(1)

with

$$H_0 = J_1^2 / 2 + \omega_2 J_2,$$

$$V_1(\theta_1) = \cos \theta_1, \quad V_2(\theta_1, \theta_2) = \cos(\theta_1 - \theta_2), \quad (2)$$

where λ_1 , λ_2 are the perturbation parameters and we assume $\omega_2 > 0$. In this paper, we consider the case $\lambda_1 = \lambda_2 = \lambda$ and we assume $\lambda \ll 1$. An extension to the case $\lambda_1 \neq \lambda_2$ is straightforward. This Hamiltonian has two primary resonances located at $J_1=0$ and $J_1=\omega_2$, respectively, in the phase space [see Fig. 1(a)]. The domain of the phase space variables are given by $-\infty < J_1 < \infty$, $0 < J_2$ for the generalized momenta, and $0 \leq \theta_i < 2\pi$, i=1,2 for the "angle" variables. Although we only consider the particular Hamiltonian (2) in this paper, one can see that our construction can be applied to more general Hamiltonian systems with more than two resonance



FIG. 1. The stroboscopic plot of our system with λ =0.01 show the onset of chaos as the separation of the resonances ω_2 decreases. The orbits of the system are plotted at $t=2\pi n/\omega_2, n=1,2,\cdots$.

terms and systems with more than two degrees of freedom.

Despite its simplicity, this Hamiltonian displays the typical features of the onset of chaos as shown in Fig. 1. In fact, the Hamiltonian (2) has been considered by many authors in the past such as Chirikov [28], Escande [29], Chandre and Jauslin [30] and has proven to be a good platform to study the transition to chaos [31]. However, these considerations were all based on the trajectory point of view in which information of the system is extracted from the phase space structure. In this paper, we will analyze the dynamics on the level of ensemble based on the Liouville equation.

In Sec. II, we will briefly review the Liouvillian formalism and the resolvent formalism of the time-dependent perturbation analysis. The asymptotic perturbation analysis will be applied to the single resonance case in Sec. III and to the interference between resonances in Sec. IV. In Sec. V, we will discuss the broken time symmetry of the most secular contributions. Finally, the relation of the Chirikov overlapping criterion and our results will be commented on in Sec. VI.

II. LIOUVILLIAN FORMALISM

On the level of ensemble, we consider the time evolution of the probability density $\rho(\vec{J}, \vec{\theta}, t)$ [with $\vec{J} = (J_1, J_2)$ and $\vec{\theta}$ $=(\theta_1, \theta_2)$] satisfying the Liouville equation [5]

$$i\frac{\partial \rho(\vec{J},\vec{\theta},t)}{\partial t} = L\rho(\vec{J},\vec{\theta},t), \qquad (3)$$

where

$$L = L_0 + \lambda \,\delta L_1 + \lambda \,\delta L_2 \tag{4}$$

is the Liouville operator defined by the Poisson bracket $L=i\{H, \}$. In Eq. (4), L_0 is the unperturbed Liouville operator corresponding to H_0 while δL_1 and δL_2 are the perturbations corresponding to the two resonance terms V_1 and V_2 in Eq. (1), respectively. The initial value problem of $\rho(\vec{J}, \vec{\theta}, t)$ is solved formally in terms of the resolvent operator 1/(L-z) as [5]

$$\rho(\vec{J},\vec{\theta},t) = e^{-iLt}\rho(\vec{J},\vec{\theta},0) = \frac{-1}{2\pi i} \int_{C} dz \frac{e^{-izt}}{L-z} \rho(\vec{J},\vec{\theta},0), \quad (5)$$

where the contour *C* lies above the real axis of *z* and goes from ∞ to $-\infty$ for t>0. The time-dependent perturbation analysis can then be carried out on Eq. (5) using the geometrical expansion [5]

$$\frac{1}{L-z} = \sum_{k=0}^{\infty} (-\lambda)^k \frac{1}{L_0 - z} \left((\delta L_1 + \delta L_2) \frac{1}{L_0 - z} \right)^k.$$
(6)

Since the unperturbed motion is integrable, the eigenspectrum of L_0 can be found easily as

$$L_0 |\vec{n}\rangle = (\vec{n} \cdot \vec{\Omega}) |\vec{n}\rangle \quad \text{with} \quad \langle \vec{\theta} | \vec{n} \rangle = \frac{1}{2\pi} e^{i\vec{n} \cdot \vec{\theta}}, \tag{7}$$

where $\hat{\Omega} = \partial H_0 / \partial J = (J_1, \omega_2)$ is the unperturbed frequencies for our system, $\vec{n} = (n_1, n_2)$ is an integer vector, and we have used Dirac's bracket notation. In the following discussion, the matrix elements of the perturbed Liouville operator (∂L $= \partial L_1 + \partial L_2$)

$$\langle \vec{n} | \delta L | \vec{n}' \rangle \equiv \left(\frac{1}{2\pi} \right)^2 \int d^2 \theta e^{-i\vec{n} \cdot \vec{\theta}} \delta L e^{i\vec{n}' \cdot \vec{\theta}}, \tag{8}$$

will be used frequently, where

$$\langle n_1, n_2 | \delta L_1 | | n_1 \pm 1, n_2 \rangle = \pm \frac{1}{2} \partial_1,$$

 $\langle n_1, n_2 | \delta L_1 | n_1 \pm 1, n_2 \mp 1 \rangle = \pm \frac{1}{2} \partial_{12},$ (9)

and all other matrix elements vanish. In Eq. (9) and henceforth, we have used the notations $\partial_1 \equiv \partial/\partial J_1$ and $\partial_{12} \equiv \partial/\partial J_1 - \partial/\partial J_2$.

As mentioned in the Introduction, we will consider the time evolution of the expectation value of observables for SPS in order to overcome the small denominator problem. For simplicity, we will consider in this paper observables that only depend on the momentum variables [i.e., $A = A(\vec{J})$ so that A is in the $|\vec{0}\rangle\langle\vec{0}|$ subspace of the Fourier expansion], as well as initial probability densities that are independent of

the action variables, i.e., $\rho(\vec{J}, \vec{\theta}, t=0) = \rho_0^{-1} (\vec{J}, t=0)/(2\pi)^2$ where ρ_0^{-1} is the zeroth Fourier component of the probability density

$$\rho(\vec{J},\vec{\theta},t) = \left(\frac{1}{2\pi}\right)^2 \sum_{\vec{n}} \rho_{\vec{n}}(\vec{J},t) e^{i\vec{n}\cdot\vec{\theta}}.$$
 (10)

We also assume that $A(\vec{J})$ and $\rho_0(\vec{J},t=0)$ are smooth enough in J_1 so that the higher-order derivatives of these functions with respect to J_1 do not give significant contributions in the perturbation expansion. We further assume that $\rho_0(\vec{J},t=0)$ vanishes at the boundary of the domain of \vec{J} .

With the above assumptions, and using Eqs. (5) and (6), the expectation value $\langle A(\vec{J}) \rangle_t$ is given by

$$\begin{split} \langle A(\vec{J}) \rangle_{t} &= \frac{-1}{2\pi i} \int d^{2}J \int_{C} dz e^{-izt} A(\vec{J}) \sum_{k=0}^{\infty} (-\lambda)^{k} \sum_{\vec{n}^{[1]}, \vec{n}^{[2]}, \dots, \vec{n}^{[k-1]}} \frac{1}{z^{2}} \\ &\times \langle \vec{0} | \, \delta L | \vec{n}^{[k-1]} \rangle \frac{1}{\vec{n}^{[k-1]} \cdot \vec{\Omega} - z} \langle \vec{n}^{[k-1]} | \, \delta L | \vec{n}^{[k-2]} \rangle \\ &\times \frac{1}{\vec{n}^{[k-2]} \cdot \vec{\Omega} - z} \cdots \langle \vec{n}^{[2]} | \, \delta L | \vec{n}^{[1]} \rangle \\ &\times \frac{1}{\vec{n}^{[1]} \cdot \vec{\Omega} - z} \langle \vec{n}^{[1]} | \, \delta L | \vec{0} \rangle \rho_{\vec{0}}(\vec{J}, 0), \end{split}$$
(11)

where we have inserted complete sets of eigenstates of the unperturbed Liouville operator. This expression will be the starting point of our asymptotic perturbation analysis discussed in the following sections.

Since single resonance systems are integrable, one can expect that nonintegrability of multiresonance systems comes from the interference between the resonances. Therefore, it is convenient to consider the two contributions separately in order to contrast their properties. This is done by dividing the time evolution of the ensemble average $\langle A(\vec{J}) \rangle_t$ into two parts; the single resonance part and the resonance interference part. The single resonance part consists of terms in Eq. (11) which contain either δL_1 or δL_2 but not both, and the resonance interference part consists of terms involving both δL_1 and δL_2 .

III. CONTRIBUTIONS FROM SINGLE RESONANCE

We first consider the single resonance part. From Eq. (11), one can easily verify that the zeroth-order contribution in λ is the unperturbed motion $\langle A(\vec{J}) \rangle_t^{(0)} = \langle A(\vec{J}) \rangle_{t=0}$, where the superscript (0) indicates the order of approximation. On the other hand, since an odd number of transitions from $|\vec{0}\rangle$ to $|\vec{0}\rangle$ is forbidden by the allowable transition of the matrix elements (9), we conclude that all odd-order contributions vanish in Eq. (11). Therefore, the first nontrivial contribution comes in second order.

A. Second-order contribution

In second order, one can see from the nonzero matrix element (9) that all possible transitions belong to the single resonance part involving either δL_1 or δL_2 . To show how the secular effect is evaluated, let us first look at the transitions involving δL_1 only $(|\vec{0}\rangle \leftarrow |\pm 1, 0\rangle \leftarrow |\vec{0}\rangle)$. The corresponding contribution to $\langle A(\vec{J}) \rangle_t^{(2)}$ is given by Eq. (11) as

$$\begin{split} \frac{\lambda^2}{2\pi i} \int d^2 J \int_C dz e^{-izt} A(\vec{J}) \\ & \times \sum_{n=\pm 1} \frac{1}{z^2} \langle \vec{0} | \delta L_1 | n, 0 \rangle \frac{1}{nJ_1 - z} \langle n, 0 | \delta L_1 | \vec{0} \rangle \rho_0^-(\vec{J}, 0) \\ &= \frac{-\lambda^2}{2^2\pi i} \int dz \frac{e^{-izt}}{z^2} \int d^2 J A(\vec{J}) \partial_1 \left[\frac{1}{J_1 - z} - \frac{1}{J_1 + z} \right] \partial_1 \rho_0^-(\vec{J}, 0), \end{split}$$
(12)

where we have used the explicit form of the matrix elements (9). It is well known that the secular effect comes from the pole contribution at $z=i0^+$ [5] and the factor $\lim_{z\to i0^+} [1/(J_1)$ $(-z)-1/(J_1+z)=2\pi i \delta(J_1)$ becomes a distribution in this limit [32]. Thanks to the momentum variable integration, the δ function can be integrated and gives a definite value even though the denominator vanishes at the resonance point J_1 =0. The predominate time dependence of Eq. (12) is then given by the secular contribution that comes from the residue of the second-order pole z^{-2} , i.e., $\lambda^2 \int_C dz e^{-izt}/z^2 \sim \lambda^2 t$, since it grows asymptotically in time. Note that this secular time dependence $\lambda^2 t$ of SPS is the same as the one in the $\lambda^2 t$ expansion of LPS. We will see shortly that a significant deviation from LPS starts from the λ^4 calculation. We also note that this consideration of the resonance effect is only possible on the ensemble level where we integrate over the momentum variables.

The secular effect of the transition involving δL_2 can be estimated in a similar way. Here we summarize the result from all λ^2 transitions as

$$\langle A(\vec{J}) \rangle_{t}^{(2)} \approx \frac{-\lambda^{2} t \pi}{2} \left[\int dJ_{2} [\partial_{1} A(\vec{J})] [\partial_{1} \rho_{\vec{0}}(\vec{J}, 0)] \right|_{J_{1}=0} + \int dJ_{2} [\partial_{12} A(\vec{J})] [\partial_{12} \rho_{\vec{0}}(\vec{J}, 0)] \left|_{J_{1}=\omega_{2}}\right],$$
(13)

where \asymp means the most secular terms and any other contributions have been ignored.

B. Higher-order contributions

As mentioned before, a stronger secular effect is obtained in SPS than in LPS. To understand the origin of the stronger secular effect, we consider the λ^4 contribution and look at a representative transition generated only by δL_1

$$\vec{0} \stackrel{\delta L_1}{\leftarrow} |\pm 1, 0\rangle \stackrel{\delta L_1}{\leftarrow} |\vec{0}\rangle \stackrel{\delta L_1}{\leftarrow} |\pm 1, 0\rangle \stackrel{\delta L_1}{\leftarrow} |\vec{0}\rangle.$$
(14)

From Eq. (11), its contribution to $\langle A(\vec{J}) \rangle_t^{(4)}$ is given by

$$\frac{\lambda^{4}}{2^{3}\pi i} \int_{C} dz \frac{e^{-izt}}{z^{3}} \left[\int d^{2} J A(\vec{J}) \right] \\ \times \partial_{1} \left(\frac{1}{J_{1} - z} - \frac{1}{J_{1} + z} \right) \partial_{1}^{2} \left(\frac{1}{J_{1} - z} - \frac{1}{J_{1} + z} \right) \left[\partial_{1} \rho_{0}(\vec{J}, 0), \right]$$

$$(15)$$

where the factor z^{-3} comes from the zeroth states $|0\rangle$ in the transitions (14). It is natural to ask if the secular effect of Eq. (15) comes from the third-order pole z^{-3} similar to the case of λ^2 calculation discussed previously. If it would be the case, we would obtain the most secular effect of $\lambda^4 \int_C dz e^{-izt}/z^3 \sim \lambda^4 t^2$. However, a closer look at Eq. (15) reveals a higher-order singularity z^{-6} and leads to a much stronger secular effect of $\lambda^4 \int_C dz e^{-izt}/z^6 \sim \lambda^4 t^5$. In fact, the extra pole comes from the product of the propagators in Eq. (15)

$$\left(\frac{1}{J_1-z} - \frac{1}{J_1+z}\right)\partial_1^2 \left(\frac{1}{J_1-z} - \frac{1}{J_1+z}\right) = \frac{2z}{J_1^2-z^2}\partial_1^2 \frac{2z}{J_1^2-z^2}.$$
(16)

For simplicity, let us first consider the product $[z/(J_1^2-z^2)]$ $\times [z/(J_1^2-z^2)]$ (i.e., without the derivatives ∂_1^2). If we would miscount the pole in Eq. (15) as z^{-3} , then one would encounter the product of δ function $[z/(J_1^2-z^2)][z/(J_1^2-z^2)]$ $\rightarrow (i\pi)^2 \delta(J_1) \delta(J_1)$ [by using $\delta(J_1) \propto z/(J_1^2-z^2)$ in the limit $z \rightarrow i0^+$ as before] which diverges even under the integration over the momentum variables. However, this problem can be solved if we carefully extract additional poles from the product of the propagators, i.e., by considering

$$\frac{z}{J_1^2 - z^2} \frac{z}{J_1^2 - z^2} = \frac{1}{z} \left[\frac{z^3}{(J_1^2 - z^2)^2} \right].$$
 (17)

Now if we use another expression of the δ function $\delta(J_1) \propto z^3/(J_1^2-z^2)^2$ in the limit $z \rightarrow i0^+$ [32], we can avoid the product of δ function by extracting the extra pole z^{-1} .

Furthermore, the derivative operators ∂_1^2 in Eq. (16) will give rise to additional poles of z^{-2} since they act on J_1 and increase the power of the denominator in Eq. (16) by 2. Therefore, all together $[z^{-3}$ from the zeroth state $|\vec{0}\rangle$, z^{-1} from the product of two propagators in Eq. (17) and z^{-2} from the derivatives] we obtain the sixth-order pole z^{-6} , which results in stronger secular effects of $\lambda^4 t^5$, $\lambda^4 t^4$, \cdots in SPS. For large time scale, the most secular term of $\lambda^4 t^5$ is dominated.

Although the above procedure extracting the secular effects is transparent in understanding the origin of the extra singularities of the resonance, it is not conveniently applied to higher-order calculations because identifying the δ function from the product of propagators could be highly nontrivial. Therefore, we developed a different approach to extract the same secular effect as discussed above. To illustrate this method, we again consider the transition (14). The same result can be obtained by first evaluating the residue of the factors (16) in Eq. (15) at the poles on either the upper or

lower-half complex J_1 plane. In the following calculations, we will choose the poles on the upper-half plane. Thus, we evaluate the secular effect of Eq. (15) by

$$\frac{\lambda^{4}}{2^{3}\pi i}(2\pi i)^{2}\operatorname{Res}_{z=i0^{+}}\left\{\frac{e^{-izt}}{z^{3}}\operatorname{Res}_{J_{1}=z}\left[\int dJ_{2}A(\vec{J})\partial_{1}\left(\frac{1}{J_{1}-z}-\frac{1}{J_{1}+z}\right)\partial_{1}^{2}\left(\frac{1}{J_{1}-z}-\frac{1}{J_{1}+z}\right)\partial_{1}\rho_{0}^{-}(\vec{J},0)\right]\right]\right\}$$

$$\approx \frac{\lambda^{4}}{2^{3}\pi i}(2\pi i)^{2}\operatorname{Res}_{z=i0^{+}}\left[\frac{e^{-izt}}{z^{3}}\left(\frac{-1}{2z^{3}}\int dJ_{2}[\partial_{1}A(\vec{J})][\partial_{1}\rho_{0}^{-}(\vec{J},0)]\right|_{J_{1}=z}\right)\right]$$

$$\approx \frac{-\lambda^{4}t^{5}\pi}{2^{2}5!}\int dJ_{2}[\partial_{1}A(\vec{J})][\partial_{1}\rho_{0}^{-}(\vec{J},0)]\left|_{J_{1}=0}\right,$$
(18)

where the extra pole of z^{-3} is automatically generated from the residue of the J_1 integration at the resonance point. Therefore, we obtained the same secular time dependence as our previous consideration.

One can repeat a similar calculation for all other possible transitions with arbitrary power of λ . Here, we summarize the most secular effects for the single resonance part of our system. The detailed derivation is given in Appendix A. The result is

where a_m is determined by the residues of the propagators [Eq. (18)]

$$\sum_{\{\vec{n}\}}^{\prime} \operatorname{Res}_{J_{1}=\{\xi\}} \left[\frac{1}{\vec{n}^{[2m-1]} \cdot \vec{\Omega} - z} \partial_{1} \frac{1}{\vec{n}^{[2m-2]} \cdot \vec{\Omega} - z} \partial_{1} \cdots \partial_{1} \frac{1}{\vec{n}^{[1]} \cdot \vec{\Omega} - z} \right] = \frac{a_{m}}{z^{4m-4}}.$$
(20)

ger resonance effects than LPS.

Here $\Sigma'_{\{\vec{n}\}}$ means summation over the most secular transitions defined in Appendix A, and $\{\xi\}$ are poles of the propagators $(\vec{n}^{[i]} \cdot \vec{\Omega} - z)^{-1}$ on the upper-half complex J_1 plane.

For small λ , Eq. (19) gives a predominant contribution to $\langle A(\vec{J}) \rangle_t$ for $t \sim 1/\sqrt{\lambda}$. Therefore, we obtain a stronger secular contribution of $\lambda^{3/2}(\sqrt{\lambda}t)^{4m-3}$ for SPS instead of the $(\lambda^2 t)^m$ contribution in LPS. Since the secular contributions come



FIG. 2. Comparison of the most secular series (19) with the numerical simulation and the integral representation (22) for $A(\vec{J}) = J_1$.

spect to J_1 do not give significant contributions. The numerical result is obtained by solving the full

Hamilton's equation of motion with an ensemble of trajectories distributed according to the above choice of the probability density. We have chosen 4000 samples to calculate the ensemble average of J_1 . We see that Eq. (19) gives a good approximation to the full dynamics up to $t \approx 5/\sqrt{\lambda} = 50$.

from the resonance effects, this implies that SPS have stron-

secular effects (calculated up to λ^{16}) of the single resonance

part (19) with the numerical simulation for $A(J)=J_1$ and

 $\rho_{\vec{0}}(\vec{J},t=0)/(2\pi)^2 = (\sigma\sqrt{\pi})^{-1}e^{-(J_1-J_{10})^2/\sigma^2}\delta(J_2-J_{20})$ with λ

=0.01, J_{10} =0.3, J_{20} =1.0, and σ =1.0. This choice of $\sigma \gg \sqrt{\lambda}$

ensures that $\rho_0(J,t=0)$ is wide enough to cover both primary resonance regions. It also guarantees that $\rho_0(\vec{J},t=0)$ is

smooth enough so that its higher-order derivatives with re-

In Fig. 2, we show the comparison between the most

In spite of the good agreement between our theoretical result and the numerical simulation in a certain domain of time, there are three major discrepancies as shown in Fig. 2. First, a large discrepancy for t > 50 is due to the truncation of the most secular series at λ^{16} . Second, the slight deviation of

the most secular contributions above the numerical result comes from the fact that we have not taken into account the resonance interference in our theoretical expression (19). Third, the flat part of the numerical curve at t=0 (which is known as the Zeno effect [33]) has not been recovered by our theoretical calculation, as the Zeno effect is known to come from nonsecular contributions.

In order to improve the approximation for time scales much longer than $5/\sqrt{\lambda}$, we need to evaluate terms in Eq. (19) much higher order than λ^{16} . However, this is not an easy task since the general expression of the coefficient a_m is very complicated. Nevertheless, by using the fact that the single resonance contribution comes from the integrable part of the Hamiltonian, one can obtain a compact expression of the series expansion (19) in an integral form. To obtain this integral representation, we note that the integrable part is essentially a simple pendulum where the solution of the equations of motion is given by elliptic functions. Using this exact solution, one can then expand $\langle A(\vec{J}) \rangle_t$ perturbatively in λ in the form as

$$\langle A(\vec{J}) \rangle_t - \langle A(\vec{J}) \rangle_{t=0} = \lambda^{3/2} f_{3/2}(\tau) + \lambda^2 f_2(\tau) + O(\lambda^{5/2}),$$
(21)

where $\tau \equiv \sqrt{\lambda}t \sim O(1)$ in the time scale of $t \sim 1/\sqrt{\lambda}$, and $f_{n/2}(\tau)$ with $n \geq 3$ are functions expressed by the phase space integration of elliptic functions. Therefore, in the asymptotic limit considered in this paper (i.e., with $t \to \infty$, $\lambda \to 0$, and keeping $\tau = \sqrt{\lambda}t$ finite), the predominant contribution to Eq. (21) is given by $\langle A(\vec{J}) \rangle_t \approx \langle A(\vec{J}) \rangle_{t=0} + \lambda^{3/2} f_{3/2}(\tau)$. Here we present the explicit expression of $f_{3/2}(\tau)$ as the integral representation of Eq. (19) with $A(\vec{J}) = J_1$ and $\rho_0(\vec{J}) = \rho_1(J_1) \delta(J_2 - J_{20})$

$$\langle J_1 \rangle_t \approx \int dJ_1 J_1 \rho_1(J_1) - \frac{2^{7/2}}{3} \pi \lambda^{3/2} \rho_1'(J_1) \left[1 + \int_1^\infty dx x^2 \left(\frac{\pi \sqrt{x^2 + 1}}{2x K[\sqrt{2}/(1 + x^2)]} - 1 \right) \right] + 2^3 \lambda^{3/2} \rho_1'(J_1) \int_0^1 dx \int_{-2K(\sqrt{x})}^{2K(\sqrt{x})} dbx \ \operatorname{cn}(\tau + b, \sqrt{x}) \operatorname{cn}(b, \sqrt{x}) + 2^{5/2} \lambda^{3/2} \rho_1'(J_1) \int_0^1 dx \int_{-\pi}^{\pi} db \frac{2\sqrt{2 - x^2}}{x^2} \times \left[\frac{2K(x)}{\pi} \operatorname{dn}[K(x)b/\pi + \tau/x, x] - 1 \right] \left[\sqrt{\frac{2}{2 - x^2}} \ \operatorname{dn}[K(x)b/\pi, x] - 1 \right],$$

$$(22)$$

where K(x) is the complete elliptic integral, cn(u,x) and dn(u,x) are the Jacobian elliptic functions, and $\rho'_1(J_1) \equiv d\rho_1(J_1)/dJ_1$. The detailed derivation of this expression will be presented in a separate paper [34]. We show in Fig. 2 the good agreement of the integral representation (22) and the numerical result for time scales much longer than $5/\sqrt{\lambda}$.

IV. INTERFERENCE BETWEEN RESONANCES

In this section we consider the contributions from the resonance interference. We will see that the interference leads to new poles on the complex *z* plane (besides $z=i0^+$) related to higher harmonics in the nonlinear system and gives rise to secular effects in powers of *t* as well as oscillations corresponding to higher-order resonances.

For the weakly coupled case $(\omega_2 \gg \sqrt{\lambda})$ in which the separation between the two primary resonances is large compared with the width of their separatrices, one may expect that the interference part gives a small correction to the single resonance part discussed in the preceding section. However, the consistent estimation of the interference effect is important even in the weakly coupled case, as this is the first nontrivial correction that comes from the nonintegrability of the system. In the following discussion, we will restrict our consideration to this weakly coupled case.

The interference contributions first appear in fourth order. We use the following transition as an example to demonstrate the essence:

$$\vec{0} \stackrel{\delta L_1}{\longrightarrow} |1,0\rangle \stackrel{\delta L_1}{\longleftarrow} |\vec{0}\rangle \stackrel{\delta L_2}{\longleftarrow} |-1,1\rangle \stackrel{\delta L_2}{\longleftarrow} |\vec{0}\rangle.$$
(23)

To simplify our presentation, we consider $A(\vec{J})=J_1$ and $\rho_0(\vec{J})=\rho_1(J_1)\,\delta(J_2-J_{20})$ with $\rho_1(J_1)=(4\,\pi^{3/2}/\sigma)e^{-(J_1-J_{10})^2/\sigma^2}$ as in the last section. The contribution of the transition (23) to $\langle J_1 \rangle_t^{(4)}$ is then given by [see Eqs. (11) and (9)]

$$\frac{-\lambda^4}{2^5\pi i} \int_C dz \frac{e^{-izt}}{z^3} \int dJ_1 \frac{1}{J_1 - z} \partial_1^2 \frac{1}{-J_1 + \omega_2 - z} \partial_1 \rho_1(J_1),$$
(24)

where the J_2 integration has been carried out using integration by parts.

We now apply the procedure discussed in the last section. The secular effect of Eq. (24) can be obtained by evaluating the residue of the poles on the upper-half plane of J_1 as

$$\frac{-\lambda^{4}}{2^{4}} \int_{C} dz \frac{e^{-izt}}{z^{3}} \operatorname{Res}_{J_{1}=z} \left[\frac{1}{J_{1}-z} \partial_{1}^{2} \frac{1}{-J_{1}+\omega_{2}-z} \partial_{1}\rho_{1}(J_{1}) \right] \\ \approx \frac{-\lambda^{4}}{2^{4}} \int_{C} dz \frac{e^{-izt}}{z^{3}} \left[\frac{2\rho_{1}'(J_{1})}{(\omega_{2}-2z)^{3}} + \frac{2\rho_{1}''(J_{1})}{(\omega_{2}-2z)^{2}} + \frac{\rho_{1}^{(3)}(J_{1})}{\omega_{2}-2z} \right] \Big|_{J_{1}=z},$$
(25)

where $\rho_1^{(i)}(J_1) \equiv \partial^i \rho_1(J_1) / \partial J_1^i$. In Eq. (25), a new pole appears at $z = \omega_2/2$ in contrast to the single resonance case [see, e.g., Eq. (18)]. This new pole comes from the interference between the propagators $(J_1-z)^{-1}$ and $(-J_1+\omega_2-z)^{-1}$. One then sees from Eq. (25) that the poles $[(\omega_2-2z)^{-n}, n = 1, 2, 3]$

lead to the secular effect with oscillations $(\lambda^4 t^2 e^{-i\omega_2 t/2}, \lambda^4 t e^{-i\omega_2 t/2}, \cdots)$ while the pole z^{-3} gives rise to secular effects in powers of t $(\lambda^4 t^2, \lambda^4 t, \cdots)$.

The secular effect with the oscillation $e^{-i\omega_2 t/2}$ can be easily related to the periodic orbit associated with the secondary resonance located at $J_1 = \omega_2/2$ for our system [see Fig. 1(a)]. This periodic orbit comes from the particular solution ($J_1 = \omega_2/2$, $\theta_1 = \omega_2 t/2$, $\theta_2 = \omega_2 t$) of the Hamilton's equation of motion, as the angular frequency $\omega_2/2$ of the angle variable θ_1 gives the oscillation $e^{-i\omega_2 t/2}$ in the secular effect. However, in the trajectory approach it is generally not easy to find higher periodic solutions of nonintegrable systems. By evaluating the secular effects in the ensemble approach, one can automatically take into account the contributions from the resonance effects of these higher periodic motions.

A similar calculation can be applied to other λ^4 transitions. After summing the contribution from all λ^4 transitions, we find that terms proportional to $\lambda^4 t^2$ cancel out and the λ^4 most secular effect of the interference part of $\langle J_1 \rangle_t$ is given by

$$-\lambda^{4}t\pi \left. \left(\frac{5\rho_{1}'(J_{1})}{2\omega_{2}^{4}} + \frac{5\rho_{1}''(J_{1})}{4\omega_{2}^{3}} + \frac{3\rho_{1}^{(3)}(J_{1})}{8\omega_{2}^{2}} + \frac{\rho_{1}^{(4)}(J_{1})}{8\omega_{2}} \right) \right|_{J_{1}=0} \\ -\lambda^{4}t\pi \left. \left(\frac{5\rho_{1}'(J_{1})}{2\omega_{2}^{4}} - \frac{5\rho_{1}''(J_{1})}{4\omega_{2}^{3}} + \frac{3\rho_{1}^{(3)}(J_{1})}{8\omega_{2}^{2}} - \frac{\rho_{1}^{(4)}(J_{1})}{8\omega_{2}} \right) \right|_{J_{1}=\omega_{2}} \\ - \left. \frac{2\lambda^{4}t\pi\rho_{1}'(J_{1})}{\omega_{2}^{4}} (e^{i\omega_{2}t/2} + e^{-i\omega_{2}t/2}) \right|_{J_{1}=\omega_{2}/2}.$$
(26)

Using the same procedure, we can calculate the most secular effects from higher-order contributions. Similarly, we find secular effect with oscillation, e.g., the λ^6 and λ^8 most secular effect are found to be $\alpha \lambda^6 t^7 (e^{i\omega_2 t} + e^{-i\omega_2 t})/\omega_2^2$ and $\alpha \lambda^8 t^{11} (e^{i\omega_2 t} + e^{-i\omega_2 t})/\omega_2^2$, respectively. In Fig. 3, we show the secular effects of the λ^4 , λ^6 , and λ^8 contributions for $\sigma = 1.0$, $J_{10} = 0.3$, $J_{20} = 1.0$, $\omega_2 = 0.8$, and $\lambda = 0.01$. We see that the λ^4 contribution with oscillation frequency $\omega_2/2$ is dominant in the time scale of $t \sim 1/\sqrt{\lambda}$ for the interference part.

In order to compare our theoretical prediction in this section with the numerical simulation, we need to extract the contribution of interference part from the full dynamics. So we write $\langle J_1 \rangle_t$ in the form of



FIG. 3. The λ^4 , λ^6 , and λ^8 order contributions of the most secular effect for the interference part.

$$\langle J_1 \rangle_t = \langle J_1 \rangle_{t=0} + [\langle J_1 \rangle_t]_{\delta L_1} + [\langle J_1 \rangle_t]_{\delta L_2} + [\langle J_1 \rangle_t]_{\delta L_1, \delta L_2},$$
(27)

where $[\langle J_1 \rangle_t]_{\delta L_1, \delta L_2}$ represents the interference part of $\langle J_1 \rangle_t$ [i.e., terms in Eq. (11) containing both δL_1 and δL_2] while $[\langle J_1 \rangle_t]_{\delta L_1}$ and $[\langle J_1 \rangle_t]_{\delta L_2}$ denote the contribution from the single resonance part. From this relation, we see that the interference part is given by $[\langle J_1 \rangle_t]_{\delta L_1, \delta L_2} = \langle J_1 \rangle_t - [\langle J_1 \rangle_t]_{\delta L_1} - [\langle J_1 \rangle_t]_{\delta L_2} - \langle J_1 \rangle_{t=0}$.

We plot the comparison between our theoretical result (the sum of λ^4 , λ^6 and λ^8 secular effect from the interference part) and the numerical simulation in Fig. 4 with the same parametrization as in Fig. 3. In this figure, the time evolution of the ensemble average $\langle J_1 \rangle_t$ is numerically calculated by choosing 5000 samples of trajectories. On the other hand, we have used the exact analytic expression in terms of the elliptic functions for $[\langle J_1 \rangle_t]_{\delta L_i}$ with i=1,2.

V. BROKEN TIME SYMMETRY

As in the case of LPS, the secular effects of SPS found by evaluating the resonance effects break time symmetry [5]. To



FIG. 4. Comparison of theoretical prediction with numerical simulation for the interference part.

see this, let us express the most secular series (19) in terms of a "time evolution operator" $\Sigma(t)$ as

$$\langle A(\vec{J}) \rangle_t - \langle A(\vec{J}) \rangle_{t=0} \asymp \int d^2 J A(\vec{J}) \Sigma(t) \rho_{\vec{0}}(\vec{J},0),$$
 (28)

with

$$\Sigma(t) \equiv \lambda^{3/2} \pi (\partial_1 \delta(J_1) \partial_1 + \partial_{12} \delta(J_1 - \omega_2) \partial_{12})$$
$$\times \sum_{m=1}^{\infty} \frac{(-1)^m (\sqrt{\lambda} t)^{4m-3} a_m}{2^{2m-1} (4m-3)!},$$
(29)

which gives the most secular effects of the time evolution.

Let us denote the time-reversal operator by *T*. The basic properties of *T* are listed in Appendix B. Using these properties, we see that $T\vec{n}\cdot\vec{\Omega}=\vec{n}\cdot\vec{\Omega}T$, i.e., the eigenvalues of the unperturbed Liouville operator L_0 are invariant under the time-reversal operation. As a result, we have $T\delta(J_1) = \delta(J_1)T$ and $T\delta(J_1-\omega_2) = \delta(J_1-\omega_2)T$. Similarly, we have $T(n_1\partial_1+n_2\partial_2)=(n_1\partial_1+n_2\partial_2)T$ for the interaction [see Eqs. (B3)–(B5)]. Therefore, all together we have

$$T\Sigma(t) = \Sigma(t)T \neq \Sigma(-t)T.$$
(30)

On the other hand, the time-reversal symmetry of the time evolution operator $U(t) \equiv \exp(-iLt)$ is expressed by (see Appendix B)

$$TU(t) = U(-t)T.$$
(31)

Hence, the time symmetry of the most secular effect in Eq. (30) is broken in comparison to Eq. (31).

The origin of the broken time symmetry is the resonance effect which is evaluated as the δ function. The appearance of the δ function comes from the analytic continuation of the denominator into the complex plane as in the case of LPS [5], i.e.,

$$\frac{1}{\vec{n}\cdot\vec{\Omega}} \Rightarrow \frac{1}{\vec{n}\cdot\vec{\Omega}\pm i0^+} = P \frac{1}{\vec{n}\cdot\vec{\Omega}} \mp i\pi\delta(\vec{n}\cdot\vec{\Omega}), \quad (32)$$

where *P* denotes the principal part. Indeed, if Eq. (29) would have the off-resonance contribution from the principal part instead of the δ function part, we would have the same timereversal symmetry as in Eq. (31) since there is no factor of *i* in the principal part as shown in Eq. (32).

Note that the secular effects of the interference part discussed in Sec. IV also come from the effect of resonance singularities and break time symmetry. Since the order of the secular effects in λ of the interference part are different from the single resonance part, there is no way to compensate their broken time symmetric contributions. We also note that the δ function part may contribute only under the integration over the momentum variables. This implies that time symmetry is broken only on the ensemble level, but not on the level of individual trajectories.

VI. CONCLUDING REMARKS

From the results of Secs. III and IV, it is interesting to compare the most secular effect of the interference part with the single resonance part. For example, the ratio of the λ^4 secular effect of the interference part (26) to the λ^4 single resonance contribution (18) is given by

$$\left(\frac{1}{\omega_2 t}\right)^4 \sim \left(\frac{\sqrt{\lambda}}{\omega_2}\right)^4,$$
 (33)

for $t \sim 1/\sqrt{\lambda}$. Hence contribution from the interference part is a small correction in the weakly coupled case ($\omega_2 \ge \sqrt{\lambda}$). However, Eq. (33) shows that the interference part is no longer a small correction to the single resonance part in the strongly coupled case ($\omega_2 \sim \sqrt{\lambda}$).

We note that the condition $\omega_2 \sim \sqrt{\lambda}$ is exactly the same condition for the onset of global chaos analyzed by Chirikov [28] in terms of the overlapping condition of the resonances on the level of trajectory dynamics. It is interesting to find the same condition by analyzing the secular effects on the level of ensemble.

In conclusion, we have described in this paper an asymptotic perturbative approach of studying analytically the secular effects of nonintegrable small Hamiltonian systems with few degrees of freedom on the ensemble level. Furthermore, we have shown that these secular effects break time symmetry.

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APPENDIX A: DERIVATION OF EQS. (19) and (20)

Without loss of generality, we consider a generic transi- ΔL_1 ΔL_1 ΔL_1 ΔL_1 ΔL_1 ΔL_1 tion $(|\vec{0}\rangle \leftarrow |n_1^{[2m-1]}, 0\rangle \leftarrow \cdots \leftarrow |n_1^{[1]}, 0\rangle \leftarrow |\vec{0}\rangle)$ of order λ^{2m} corresponding to the resonance at $J_1=0$ in Eq. (11). Its most secular contribution to $\langle A(\vec{J}) \rangle_t^{(2m)}$ is obtained by evaluating the residues (see Sec. III B) and is given by [using the matrix element (9)] RESONANCE OVERLAP, SECULAR EFFECTS, AND...

$$(-1)^{m}(2\pi i)\left(\frac{\lambda}{2}\right)^{2m}\underset{z=i0^{+}}{\text{Res Res}} \left[\frac{e^{-izt}}{z^{2}}\int dJ_{2}[\partial_{1}A(\vec{J})]\left\{\frac{1}{n^{[2m-1]}J_{1}-z}\partial_{1}\frac{1}{n^{[2m-2]}J_{1}-z}\cdots\partial_{1}\frac{1}{n^{[1]}J_{1}-z}\right\}\partial_{1}\rho_{\vec{0}}(\vec{J},0)\right],$$
(A1)

where $\{\xi\} = \{\xi_1, \xi_2, \cdots\}$ are poles of the propagators on the upper-half complex J_1 plane. Equation (A1) shows that these poles should take the form $\xi_i = z/p_i, i=1, 2, \cdots$, where $p_i \neq 0$ are positive integers.

Note that extracting the most secular effect from Eq. (A1) means extracting the highest-order pole at $z=i0^+$. Without changing the highest-order pole structure, we proceed by moving the factor $\partial_1 \rho_0(\vec{J}, 0)$ to the front of the curly bracket. The most secular effect (A1) then becomes

$$(-1)^{m}(2\pi i)\left(\frac{\lambda}{2}\right)^{2m} \int dJ_{2}(\partial_{1}A(\vec{J}))(\partial_{1}\rho_{\vec{0}}(\vec{J},0)) \left| \operatorname{Res}_{J_{1}=0} \left[\frac{e^{-izt}}{z^{2}}\operatorname{Res}_{J_{1}=\{\xi\}}\left[\frac{1}{n^{[2m-1]}J_{1}-z}\partial_{1}\frac{1}{n^{[2m-2]}J_{1}-z}\cdots\partial_{1}\frac{1}{n^{[1]}J_{1}-z}\right]\right].$$
(A2)

We also note that the residue evaluated at the poles $J_1 = \{\xi\}$ in Eq. (A2) vanishes if all $\{\xi\}$ lie above $(n^{[i]} > 0$ for all *i*) or below $(n^{[i]} < 0$ for all *i*) the real- J_1 axis. Therefore, the most secular effects are given by transitions having both positive and negative $n^{[i]}$'s which we call the most secular transitions. For these transitions, it is easy to see that

$$\operatorname{Res}_{J_{1}=\{\xi\}}\left[\frac{1}{n^{[2m-1]}J_{1}-z}\partial_{1}\frac{1}{n^{[2m-2]}J_{1}-z}\cdots\partial_{1}\frac{1}{n^{[1]}J_{1}-z}\right]$$
$$=\frac{c_{m,\{n^{[2m-1]},\cdots,n^{[1]}\}}}{z^{4m-4}},$$
(A3)

where $c_{m,\{n^{[2m-1]},\dots,n^{[1]}\}}$ is a constant depending on the transition. By using Eq. (A3) and evaluating the residue at the pole $z=i0^+$ in Eq. (A2), we obtain Eqs. (19) and (20) by defining a_m to be the summation of the constants $c_{m,\{n^{[2m-1]},\dots,n^{[1]}\}}$ in Eq. (A3) from all most secular transitions. The terms corresponding to the resonance $J_1 = \omega_2$ in Eq. (19) can be verified by the same procedure shown above.

APPENDIX B: THE TIME-REVERSAL OPERATOR

The time-reversal operator T is antilinear [35], i.e.,

$$T(c_1\rho_1 + c_2\rho_2) = c_1^* T\rho_1 + c_2^* T\rho_2,$$
(B1)

for any complex numbers $c_{1,2}$ and functions $\rho_{1,2}$, where $c_{1,2}^*$ is the complex conjugate of $c_{1,2}$. Its actions on the time and phase space variables are given by

$$Tt = tT, \tag{B2}$$

for the time variable,

$$TJ_1 = -J_1T, \quad T\theta_1 = \theta_1T, \tag{B3}$$

for the pendulum (J_1 is momentum and θ_1 is angle),

$$TJ_2 = J_2T, \quad T\theta_2 = -\theta_2T, \tag{B4}$$

for the harmonic oscillator (J_2 is action and θ_2 is angle) and

$$Tn_1 = -n_1T, \quad Tn_2 = n_2T,$$
 (B5)

for the Fourier conjugate variables \vec{n} of the angle variables. Hence, the time-reversal operator commutes with the Liouville operator *L*

$$TL = LT, \tag{B6}$$

and the time-reversal symmetry of the time evolution operator $U(t) \equiv \exp(-iLt)$ is expressed by Eq. (31).

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