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Chaos in Liouville's equation

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An exact map of the probability distribution function for the kicked rotor is generated by solving Liouville's equation for any arbitrary initial condition and kicking strength. This solution is compared to the analogous quantum map. In this matter we compare two linear partial differential equations describing the evolution of wave functions in Hilbert space. This exact map is also compared to Chirikov's standard map generated from the canonical equations of motion. As expected, the classical map for the probability distribution function is chaotic for large kicking potentials. The practical reversibility of Liouville's equation is compared to Schrödinger's equation and the standard map.

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I. INTRODUCTION

Dynamical chaos is characterized by random motion in the absence of any noise or randomly generated parameters. Such chaotic behavior can be found in nonlinear classical systems subjected to large external potentials [1–4]; an example of such a system displaying stochastic behavior is the one-dimensional kicked rotor. The kicked rotor is essentially a rigid pendulum subject to a periodic δ-function potential. Over the past decade, the rotor has been used as a vehicle to search for chaotic behavior in the analogous quantum system (i.e., quantum rotor) [5–15]. Dynamical chaos in classical systems is characterized by the instability of orbits in phase space generated by solving Hamilton's equation of motion [1,15,16]. For a given set of initial conditions and a large kicking potential, two nearby orbits will diverge exponentially. The average rate of divergence of the trajectories is characterized by the Kolmogorov-Sinai (KS) entropy h (h should not be confused with Planck's constant) [1], or similarly Lyapunov exponents [17]. The KS entropy provides a measure for the degree of instability of a particular trajectory; it is commonly used to define the transition to chaos. A system may be considered stochastic if $h > 1$. Two consequences of classical chaos in the kicked rotor are (1) diffusion in phase space resulting in a linear growth of the energy [1,6], and (2) "practical" irreversibility of the equations of motion [10]. By practical irreversibility we mean that the equations of motion are numerically irreversible after the system has been permitted to evolve for a characteristic time. In principle, the classical system is exactly reversible; however, a computer does not have the requisite accuracy to preserve all of the information after a characteristic time.

The quantum rotor, for an identical kicking potential, does not have all of the "tell tale" signs of chaos. Unlike the classical system, the energy does not grow diffusely in time [6]. Instead, after a short time, the energy ceases to grow and oscillates about a constant value. Furthermore, the quantum system exhibits "practical" reversibility. Sheplyansky [10] showed that the quantum rotor is practically reversible. Casati and co-workers [11,12] demonstrated that the quantum one-dimensional hydrogen atom is also practically reversible, while the classical system is practically irreversible. The lack of energy growth might very well be expected. The quantum rotor has a discrete energy spectrum. Fishman and co-workers [8], show that the discrete nature of the quasienergy spectrum localizes the wave packet. They show a similarity between the localization of the quantum rotor and Anderson localization of an electron in a solid with a randomly spaced lattice.

There is an inherent problem comparing the classical and quantum system: ordinary nonlinear (nonintegrable) differential equations (canonical equations of Hamilton), describing the evolution of orbits in phase space, are used to describe the time evolution of the classical system. On the other hand, for the quantum system, a linear partial differential equation describing the evolution of probability functions (wave functions) is solved. To overcome this problem of comparing the classical and quantum system, we solve the classical Liouville equation for the kicked rotor and compare it to the solution of Schrödinger's equation (and the canonical equations of motion). Liouville's equation is a linear partial differential equation describing the time evolution of the classical probability distribution function. The solution to Liouville's equation is analogous to the Wigner representation of the quantum phase-space distribution [18,19]. Unlike the canonical equations of motion, Liouville's equation describes a finite measure of initial conditions, and since it is first order, it can be solved by adding up the orbits. However, like the equations of motion, the solution of

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Liouville's equation should be chaotic for large kicking potentials. Ford, Mantica, and Ristow in Ref. [14] also compared the solution of Liouville's equation for the Arnol'd cat to Schrödinger's equation.

In Sec. II of this paper we provide background material on Chirikov's standard map and the quantum map for the kicked rotor. In Sec. III, a map for the classical probability distribution function similar to the quantum map [6] for the wave function is generated. This temporal map relates the classical probability distribution function before and after a kick. This classical map can be used as a new tool to further study the chaotic behavior of the classical rotor. Section IV of this paper examines the reversibility of Liouville's equation. We find that for certain kicking strengths and initial conditions Liouville's equation can be numerically iterated a few kicks longer than the standard map before information is lost. For most other conditions, compared to Schrödinger's equation Liouville's equation, as expected, is practically irreversible.

II. BACKGROUND

The one-dimensional time-dependent Hamiltonian for the kicked classical rotor is [6]

$$H=\frac{I^2}{2J}+k\cos\theta\sum_{n=-\infty}^{\infty}\delta(t-nT)\ , \tag{1}$$

where I is the angular momentum, k is the strength of the kick, θ is the angle of the rotor, T is the period of the kick, n is the kick number, J is the angular momentum, $H_0=I^2/2$ is the Hamiltonian of the free rotor, and $H_{\rm int}=k\cos\theta\sum_n\delta(t-nT)$ is the interaction term. In the rest of this paper the angular momentum $J=1$. The above Hamiltonian corresponds to a rigid pendulum subject to a nonlinear potential, $V(\theta)=k\cos\theta$, which is turned on and off for a brief instant with a period T. Integrating the canonical equations of motion over one period results in the celebrated Chirikov's standard map [1]

$$\tilde{I}_{n+1}=\tilde{I}_n+K\sin\theta_n\ , \tag{2a}$$

$$\theta_{n+1}=\theta_n+\tilde{I}_{n+1}\ , \tag{2b}$$

where $K=kT$ and $\tilde{I}=IT$. For $K\ll 1$, the map (2) is integrable; a majority of the orbits in phase space lie on invariant curves. Furthermore, when $K\ll 1$, the map (2) is reversible on a computer (practical reversibility). If $K\sim 1$, the standard map is near integrable [Kol'mogorov-Arnol'd-Moser (KAM) theory] and invariant curves (also known as KAM curves) bound regions of chaos. This case ($K\sim 1$) corresponds to the transition between integrable and nonintegrable dynamics. If $K\gg 1$, all invariant KAM curves disappear and the result is near-total chaos in phase space. For this latter case, most initially close trajectories in phase space diverge exponentially. The distance between the nearby trajectories is $d=d_0e^{ht}$, where d_0 is the initial distance between orbits and h is the Kolmogorov-Sinai (KS) entropy. For the kicked rotor $h\sim\ln(K/2)$ when $K\gg 1$ [1]. Additionally, when $K\gg 1$, the angle becomes random and the energy grows according to the diffusion law $K^2t/4$. In this stochastic regime diffusion in action space can be described by a diffusion equation [20].

The instability of orbits renders the system practically irreversible; i.e., the equations of motion can only be iterated forward for a certain time (reversal time t_r) before memory of the initial condition is lost. The reversal time is a function of both the computer accuracy and the KS entropy h [21]. The reversal time is $t_r\sim\ln\varepsilon/h$, where ε corresponds to the computer accuracy and $h\sim\ln(K/2)$. As an example, with double-digit accuracy ($\varepsilon=10^{-16}$) and $K=5$, the initial conditions will be reconstructed if a time reversal is performed after 40 iterations of the standard map, but no more. After several iterations computer round-off errors prevent the reconstruction of the initial conditions. Greene [22] has shown that these round-off errors have a negligible contribution in determining the transition to global stochasticity.

We now turn our attention to the quantum kicked rotor with the Hamiltonian [6]

$$H=-\frac{\hbar^2}{2}\frac{\partial^2}{\partial\theta^2}+k\cos\theta\sum_{n=-\infty}^{\infty}\delta(t-nT)\ . \tag{3}$$

The δ-function potential makes it convenient to describe the solution of Schrödinger's equation in the form of a map [6] given by

$$A_m(t+T)=\sum_{n'=-\infty}^{\infty}J_{m-n'}(k)\exp(-in'^2T/2)A_{n'}(t)\ , \tag{4}$$

where $A_m(t+T)$ is the eigenfunction after one kick, $J_{m-n'}$ are Bessel functions of the first kind, $E_{n'}=n'^2/2$ are the eigenvalues (free energy), $A_{n'}(t)$ is the initial eigenfunction before a kick, and Planck's constant $\hbar=1$. The wave function for Schrödinger's equation is

$$\Psi(\theta,t)=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty}A_m(t)e^{im\theta}\ . \tag{5}$$

The energy of the quantum rotor

$$E=\sum_{m=-\infty}^{\infty}\frac{m^2}{2}[A_m(t)]^2 \tag{6}$$

can be compared to the energy of the classical system. In numerical experiments, Casati *et al.* [6] found that the energy of the quantum system grows diffusely for a short time at a rate comparable to the classical system, and then ceases to grow at a break time. After this break time, the energy oscillates about a fixed value and the quantum wave packet is localized in momentum space; this localization is due to the discrete nature of the quasienergy spectrum. Fishman, Grempel, and Prange [8] show that the quasienergy spectrum of the quantum rotor is discrete. They show a similarity between the localization of the quantum rotor and Anderson localization of an electron in a solid with a randomly spaced lattice.

In addition to demonstrating nondiffusive behavior for large K, the quantum map is practically reversible when compared to the classical standard map (2). In fact, as shown by Sheplyansky [10], the difference between the initial conditions before and after reversibility is compara-

ble to the accuracy of the normalization of the eigenstates which, in turn, depends on the number of eigenfunctions summed over in (5). After a certain amount of time, if a sufficient number of eigenfunctions are not selected in (5), the quantum system will not be reversible. This condition is easily checked by examining the normalization condition after each kick.

III. SOLUTION OF LIOUVILLE'S EQUATION FOR THE KICKED ROTOR

In this section we generate a map for the probability distribution function (also known as the phase-space density function) for the kicked classical rotor by solving Liouville's equation

$$i\left[\frac{\partial\rho}{\partial t}\right]=L\rho\ , \tag{7}$$

where L is the Liouville operator given by

$$L=-i\left[\frac{\partial H}{\partial I}\right]\left[\frac{\partial}{\partial\theta}\right]+i\left[\frac{\partial H}{\partial\theta}\right]\left[\frac{\partial}{\partial I}\right]\ . \tag{8}$$

In expression (8) H is the Hamiltonian of the system, I is the angular momentum, and θ is the coordinate.

We solve Liouville's equation (7) for the Hamiltonian (1) and generate a map for the probability distribution function $\rho(I,\theta,t)$ using the method outlined by Casati *et al.* [6], or that used to generate an analogous map for the quantum wave function. This map is used to calculate the exact diffusion coefficient and energy for any initial condition and kicking strength k. Rechester and coworkers [23,24] first derived an expression for the diffusion coefficient of the standard map with an external stochastic term for large k and any value of k. Abarbanel [20] used Fourier path integrals to derive the diffusion coefficients for the standard map. Ford, Mantica, and Ristow [14] also solve Liouville's equation for the Arnol'd cat.

In solving Liouville's equation, we regard the system as a free rigid rotor perturbed by δ-function potentials. We start by solving Liouville's equation for the interaction Hamiltonian

$$H_{\rm int}=k\cos\theta\sum_{n=-\infty}^{\infty}\delta(t-nT) \tag{9}$$

to relate the probability distribution function before a kick to the probability distribution function after the kick. We set $\rho(I,\theta,t)=A(\theta,t)F(I)$ and integrate Liouville's equation

$$\frac{\partial\rho}{\partial t}=\left[\frac{\partial\rho}{\partial I}\right]\left[\frac{\partial H}{\partial\theta}\right]=\left[-k\sin\theta\sum_{n=-\infty}^{\infty}\delta(t-nT)\right]\frac{\partial\rho}{\partial I} \tag{10}$$

over one kick [the $(n+1)$th] to yield the expression

$$A_\lambda^+((n+1)T,\theta)=e^{-i\lambda k\sin\theta}A_\lambda^-((n+1)T,\theta)\ , \tag{11}$$

where the $(+)$ refers to the instant just after the $(n+1)$th kick, the $(-)$ corresponds to the time just before the $(n+1)$th kick, and $F(I)=e^{i\lambda I}$. Using (11), solutions to (10) just after the $(n+1)$th kick have the form

$$\rho^+(I,\theta,(n+1)T)=\int_{-\infty}^{\infty}d\lambda e^{i\lambda I}A_\lambda^+((n+1)T,\theta)\ . \tag{12}$$

The coefficients A_λ, before and after the kick, are obtained by setting (12) equal to the solution of the free Hamiltonian ($H_0=I^2/2$) given by [25]

$$\rho(I,\theta,t)=\sum_{m=-\infty}^{\infty}C_m(I)e^{-imIt}e^{im\theta} \tag{13}$$

to yield

$$\int_{-\infty}^{\infty}d\lambda e^{i\lambda I}A_\lambda^+((n+1)T,\theta)=\sum_{m=-\infty}^{\infty}C_m(I,(n+1)T)e^{im\theta} \tag{14}$$

after the $(n+1)$th kick, and

$$\int_{-\infty}^{\infty}d\lambda e^{i\lambda I}A_\lambda^-((n+1)T,\theta)=\sum_{m=-\infty}^{\infty}C_m(I,nT)e^{-imIT}e^{im\theta} \tag{15}$$

just before the $(n+1)$th kick. After each kick, the functional form of C_m changes, thus the notation $C_m[I,(n+1)T]$, where $(n+1)T$ denotes the fact that coefficients C_m correspond to the free propagation after the $(n+1)$th kick (ultimately we will find the relation between $C_m(I,nT)$ and $C_m[I,(n+1)T]$). Fourier transforming (14) and (15) results in expressions for the coefficients A_λ given by

$$A_\lambda^+((n+1)T,\theta)=\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}dIC_m(I,(n+1)T)e^{-i\lambda I}e^{im\theta}\ , \tag{16a}$$

and

$$A_\lambda^-((n+1)T,\theta)=\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}dIC_m(I,nT)e^{-i\lambda I}e^{im\theta}e^{-imIT}\ . \tag{16b}$$

Substituting (16b) into (11) and using (12) yields the solution for $\rho^+(I,\theta,(n+1)T)$ given by

$$\rho^+(I,\theta,(n+1)T)=\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dI'd\lambda C_m(I',nT)e^{i\lambda I}\times e^{-i\lambda k\sin\theta}e^{-i\lambda I'}e^{im\theta}e^{-imI'T}\ , \tag{17}$$

where $C_m(I',nT)$ are coefficients after the nth kick. To relate these to the coefficients after the $(n+1)$th kick, we set Eq. (17) equal to the free probability distribution function immediately after the $(n+1)$th kick given by

$$\rho^+(I,\theta,(n+1)T)=\sum_{m=-\infty}^{\infty}C_m(I,(n+1)T)e^{im\theta} \tag{18}$$

to yield

$$C_l(I,(n+1)T)=\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{2\pi}dI'd\lambda\frac{d\theta}{2\pi}e^{-i\lambda k\sin\theta}e^{i\lambda I}e^{-i\lambda I'}C_m(I',nT)e^{-imI'T}e^{i(m-l)\theta}\ . \tag{19}$$

By taking advantage of the identity

$$\int_{-\infty}^{\infty}d\lambda e^{i\lambda(I-I'-k\sin\theta}=\delta(I-I'-k\sin\theta)\ , \tag{20}$$

expression (19) simplifies to

$$C_l(I,(n+1))T)=\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{2\pi}dI'\frac{\theta}{2\pi}\delta(I-I'-k\sin\theta)C_m(I',nT)e^{-imI'T}e^{i(m-l)\theta}\ . \tag{21}$$

Integrating over I' yields the final map for C given by

$$C_l(I,(n+1)T)=\sum_{m=-\infty}^{\infty}\int_0^{2\pi}\frac{d\theta}{2\pi}C_m(I-k\sin\theta,nT)\times e^{imTk\sin\theta}e^{-imIT}e^{i(m-l)\theta}\ . \tag{22}$$

Expression (22), in combination with (13), describes the time evolution of the probability distribution function over one kick or period T. This map is analogous to the Wigner representation of the quantum phase-space distribution [18]. We use the expression

$$E=\int_0^{2\pi}\int_{-\infty}^{\infty}d\theta\,dI\frac{I^2}{2}\rho(I,\theta,(n+1)T)\ , \tag{23}$$

and (13) to calculate the rotor energy given by

$$E=2\pi\int_{-\infty}^{\infty}dI\frac{I^2}{2}C_0(I,(n+1)T)\ . \tag{24}$$

Expression (24) can be used to calculate the energy after n kicks for any arbitrary initial condition; however, proper choice of initial conditions will avoid unwieldy or otherwise time-consuming numerical computations. Here, we select initial conditions having the form

$$C_0(I,0)=\frac{\delta(I)}{2\pi}\ , \tag{25}$$

where we initially excite the zeroth-order terms. The energy after the first kick is simply

$$E=\frac{k^2}{4}\ , \tag{26}$$

while the energy after the second kick is

$$E=\frac{k^2}{4}+\frac{k^2}{4}\{1-J_2(2kT)\}\ . \tag{27}$$

The expression for the energy after more than two kicks involves the quasilinear term $(k^2/4)n$, added to an infinite sum. Calculating the probability distribution function and the energy numerically to reasonable computer accuracy quickly becomes unwieldy. Fortunately, this is true for values of the kicking strength less than, or comparable to, the critical value $kT\approx 1$. For kicking strengths above this critical value, the quasilinear term $(k^2/4)n$ yields the largest contribution to the energy and thus, the infinite sum can be truncated without losing significant accuracy. As expected, for $k\gg 1$, the energy grows linearly in time with a slope $k^2/4$.

IV. REVERSIBILITY OF LIOUVILLE'S EQUATION

We now turn our attention to the reversibility of Liouville's equation. We start by integrating Liouville's equation (7) backwards, starting from the nth kick to generate a reverse map for the probability distribution function similar to expression (22). Integrating (10) backwards yields

$$A_\lambda^-((n+1)T,\theta)=e^{i\lambda k\sin\theta}A_\lambda^+((n+1)T,\theta)\ . \tag{28}$$

This expression relates the coefficients A_λ after a kick to the coefficients just before a kick. We use the expression for the probability distribution function just before the kick

$$\rho^-(I,\theta,(n+1)T)=\int_{-\infty}^{\infty}d\lambda e^{i\lambda I}e^{i\lambda k\sin\theta}A_\lambda^+((n+1)T,\theta)\ , \tag{29}$$

and the solution of the free rotor

$$\rho^-(I,\theta,(n+1)T)=\sum_{m=-\infty}^{\infty}C_m(I,nT)e^{-imIT}e^{im\theta} \tag{30}$$

to arrive at an expression for the coefficients C_l given by

$$C_l(I,nT)e^{-ilIT}=\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{2\pi}dI'd\lambda\frac{d\theta}{2\pi}e^{i\lambda k\sin\theta}e^{i\lambda I}e^{-i\lambda I'}C_m(I',(n+1)T)e^{i(m-l)\theta}\ . \tag{31}$$

Integrating the right-hand side of (31) results in a map relating the coefficients just before a kick to those after a kick:

$$C_l(I,nT)=e^{ilIT}\sum_{m=-\infty}^{\infty}\int_0^{2\pi}\frac{d\theta}{2\pi}C_m(I+k\sin\theta,(n+1)T)\times e^{i(m-l)\theta} \tag{32}$$

The initial conditions can be reassembled after repeated applications of the map (32).

Numerical experiments were carried out with the forward (22) and the reverse (32) maps to compare the practical reversibility of the standard map, Liouville's equation, and Schrödinger's equation. Numerically, the classical map (22) is more complex than its quantum counter-

part. The integral over θ in the quantum map reduces down to a Bessel function of the first kind which greatly simplifies the numerical task. On the other hand, after each iteration of the classical map (22), the integral must be evaluated numerically with reasonable accuracy which significantly adds to the computation time. Thus, in order to reduce the computation time and, at the same time, preserve reasonable accuracy, a kicking strength $k=3000$ was used. Numerical experiments were carried out by calculating the quantum energy using (6) and classical energy using (2) and (24) for 4 kicks and then performing a time reversal. As shown in Fig. 1 the classical map (2) fails the reversibility test (the initial condition is not reproducible) after four kicks, while the solution to Liouville's and Schrödinger's equation is reversible for the initial conditions and kicking strength given above. In fact, the initial conditions are reassembled with the requested accuracy. We used single precision (eight-digit) accuracy in calculating the energy from the standard map while only three-digit accuracy was used in calculating the energy from the map (22) and (32); accuracy was verified after each kick by checking the normalization condition. For this particular case it appears that Liouville's equation contains more information than the standard map for just a few kicks. This difference is interesting and requires further investigation. This numerical evidence does not imply that Liouville's equation is more or less reversible than the standard map. First of all, for more than four kicks, unlike Schrödinger's equation, Liouville's equation is no longer practically reversible. We have repeated the numerical experiments with other initial conditions and kicking strengths and found that for many cases Liouville's equation is just as practically irreversible as the standard map. However, the condition for reversibility of Liouville's equation is similar to the quantum case. Namely, the accuracy of reversibility depends on the number of eigenfunctions summed over in the map (22) and (32). The classical map (22) is numerically more complicated than the quantum map (4). It would be very difficult to carry out the reversibility experiment for longer times; the number of eigenfunctions we have to sum over in (22) and (32) in order to guarantee reversibility increases exponentially with time and at some point becomes numerically unwieldy.

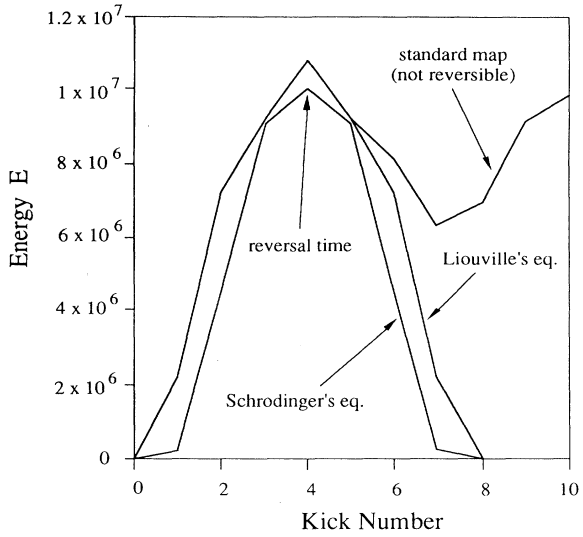

FIG. 1. Reversibility of Liouville's Equation for $k=3000$ and $T=1$. Numerical experiments were carried out by calculating the quantum energy using (6) and classical energy using (2) and (24) for four kicks and then performing a time reversal. For this set of conditions Liouville's equation and Schrödinger's equation are reversible after a few kicks.

V. CONCLUSION

Liouville's equation is a linear, integrable partial differential equation describing the time evolution of the probability distribution function. Solving Liouville's equation is inherently the same as solving the equations of motion except that one single equation is used to describe the evolution of orbits in phase space. Liouville's equation is comparable to Schrödinger's equation since it is a linear partial differential equation describing the evolution of wave functions in Hilbert space. In this paper we have generated a map for the classical probability distribution function of the one-dimensional kicked rotor by solving Liouville's equation. We have compared this solution to the solution of both Schrödinger's equation and the classical canonical equations of motion (the standard map), the solution to Liouville's equation is chaotic even though it is a linear equation; therefore, as stated by Ford, Mantica, and Ristow [14], linearity will not preclude chaotic behavior. For large k, the instability of orbits in phase space results in a diffusive growth of energy. With regard to reversibility, we find that compared to Schrödinger's equation, Liouville's equation is practically irreversible on a computer. After several iterations nearly an infinite number of eigenfunctions must be summed over to guarantee reversibility. However, we have found that for a few cases, Liouville's equation appears to be "more reversible" than the standard map (even for just a few iterations).

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