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A Semiclassical Theory of a Dissipative Henon–Heiles System

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A semiclassical theory of a dissipative Henon–Heiles system is proposed. Based on $\hbar$-scaling of an equation for the evolution of the Wigner quasiprobability distribution function in the presence of dissipation and thermal diffusion, we derive a semiclassical equation for quantum fluctuations, governed by the dissipation and the curvature of the classical potential. We show how the initial quantum noise gets amplified by classical chaotic diffusion, which is expressible in terms of a correlation of stochastic fluctuations of the curvature of the potential due to classical chaos, and ultimately settles down to equilibrium under the influence of dissipation. We also establish that there exists a critical limit to the expansion of phase space. The limit is set by chaotic diffusion and dissipation. Our semiclassical analysis is corroborated by numerical simulation of a quantum operator master equation.

KEY WORDS: Dissipative quantum system; semiclassical approximation; classical chaos; Henon–Heiles Hamiltonian.

I. INTRODUCTION

The influence of dissipation on quantum dynamics of classically chaotic systems has been one of the key issues in nonlinear dynamics today. The dynamical way of dealing with dissipation is to consider a system-heat bath model which has been the cornerstone for understanding dissipative processes[(1)] in a wide range of physical disciplines,[(2)] such as, condensed matter physics, quantum optics, chemical dynamics etc. The theoretical development in this regard is welldocumented in the literature.[(2–6)] When the system, in question, is classically chaotic, one envisages a variety of rich physics[(7–20)] concerning localization and its suppression, quantum measurement problem, irreversibility, relaxation, decoherence etc. The inferences

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drawn from these are sometimes extended to the question of generic quantum chaos. For example, a dissipative quantum system exhibting chaos in its classical limit was constructed by coupling the quantum kicked rotor to a reservoir to obtain dissipative quantum standard map by Dittrich and Graham.[7] It was observed that even weak damping is capable of disrupting dynamical localization which suppresses chaotic motion in the conservative standard map and thus restores diffusion in action variable in the timescale of classical relaxation. The effect of quantum correlation on classical chaotic behaviour had been illustrated by Sundaram and Milonni[8] by considering a kicked quantum system coupled to a reservoir. An appropriate choice of potential results in a logistic map with self-consistently generated quantum correlations. It has been observed that at intermediate range of dissipation an irregular behaviour is induced by quantum correlations even when the classical limit is regular. Based on an analysis of quantum Brownian motion in d-dimensions using the unified model for diffusion localization and dissipation, Choen[20] has proposed a semiclassical strategy at low temperature using Feynman–Vernon propagator scheme. It has been demonstrated that different mechanisms for dephasing emerge for ergodic and nonergodic motions. In another issue Bonilla and Guinea[15] have studied a simple model having quantum and classical degrees of freedom in presence of dissipation. The emergence of chaos in an open quantum system has also been considered by Spiller and Ralph.[16]

The majority of the studies considered above are based on maps, (such as, standard map or logistic map) which have been the testing ground for various theories of chaos. We construct here a dissipative version of a two-degree-of-freedom continuous system—the Henon–Heiles model,[21–23] to study the evolution of a quantum system in presence of dissipation and thermal diffusion. The Henon–Heiles model captures the essential generic features of classical chaos in nonintegrable systems and has been widely applied in the context of astronomy and chemical dynamics over the last several decades.[21–23] Based on suitable $\hbar$-scaling of Wigner equation which incorporates the effect of dissipation and thermal diffusion, we formulate a semiclassical dynamics which is governed by dissipation and curvature of the classical potential. The stability of classical motion is determined by the nature of curvature of the potential which in the chaotic regime can be considered to be a stochastic process.[24, 25] An appropriate treatment of this stochastic process in terms of the theory of multiplicative noise yields a Fokker–Planck equation of motion for Wigner-function. We design the initial conditions in terms of minimum uncertainty wave packets to maximize the classical-quantum correspondence and show how the initial wave packet corresponding to a chaotic trajectory evolves in time, and how the initial quantum noise (inherent in minimum uncertainty of wave packet) associated with it gets amplified by intrinsic classical stochasticity at the begining to eventually settle down to equilibrium under the influence of dissipation. We establish that there exists a critical limit to the expansion of phase space. The limit is set by chaotic diffusion and dissipation. Our semiclassical analysis is supplemented by quantum simulation of the operator master equation to verify the basic theoretical propositions.

The outlay of the paper is as follow: In Section II we introduce the quantum operator master equation and the Wigner function equation for an open system. $\hbar$-scaling of the Wigner equation results in a semiclassical equation governed by the dissipation due to the surroundings and the curvature of the potential. This is followed by van Kampen's treatment of multiplicative noise[26, 27] to deal with stochastic fluctuations of the curvature of the potential which leads to a Fokker–Planck equation. In Section III the Fokker–Planck equation is adapted to Henon–Heiles system followed by a detailed analysis of the problem. In Section IV a numerical simulation of the operator master equation has been carried out to verify the theorerical propositions. The approximations and their validity with a summary of the main results have been discussed in Section V.

II. CHAOTIC EVOLUTION OF AN OPEN SYSTEM; GENERAL ASPECTS

A. Quantum Dynamics

To study[2] the evolution of a quantum system in presence of weak dissipation and thermal diffusion we first consider the Hamiltonian of an N-degree-of-freedom system H_0.

$$H_0 = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + V(\{q_i\}), \qquad i = 1 \cdots N \tag{1}$$

where $\{q_i, p_i\}$ represents the coordinates and momenta of the N-degree-of-freedom system. $V(\{q_i\})$ is a nonlinear potential such that the classical version of H_0 admits of chaos.

The bare system is then coupled to an environment modeled by a reservoir of harmonic oscillators, governed by the following total Hamiltonian

$$H = H_0 + \hbar \sum_j^{\infty} \Omega_j b_j^{\dagger} b_j + \hbar \sum_j^{\infty} [k(\Omega_j)\, b_j + k^*(\Omega_j)\, b_j^{\dagger}]\, q \tag{2}$$

where b_j ($b_j^\dagger$) denotes the annihilation (creation) operator for the harmonic oscillators which comprise a bath. The third term represents the linear coupling of one of the selected degrees of freedom (through co-ordinate q) of the system to the bath. $k(\Omega_j)$ signifies the coupling constant.

It is convenient to invoke first the rotating wave approximation (RWA). After appropriate elimination of reservoir variables in the usual way using Born and Markov approximations we are lead to the following standard reduced density matrix equation for the evolution of the system,[2]

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H_0, \rho] + \frac{\gamma}{2}(2a\rho a^\dagger - a^\dagger a\rho - \rho a^\dagger a) + D(a^\dagger \rho a + a\rho a^\dagger - a^\dagger a\rho - \rho a a^\dagger) \tag{3}$$

Here we have expressed the system operators q, p (for $N = 1$) in terms of a harmonic oscillator operators a (annihilation) and $a^\dagger$ as $q = (1/\sqrt{2m\omega})(a + a^\dagger)$ and $p = i(\sqrt{m\omega/2})(a - a^\dagger)$. Note that the harmonic oscillator characterized by frequency ω has nothing to do with the reservoir of harmonic oscillators. In the derivation above, one uses a broad band spectral density function for the reservoir evaluated at ω to realize the damping constant γ as $2\pi\,|k(\omega)|^2\, g(\omega)$ within a Markovian scheme. D ($= \bar{n}\gamma$) is the diffusion coefficient and $\bar{n}$ ($= [\exp(\hbar\omega/kT) - 1]^{-1}$) refers to the average thermal photon number of the reservoir. The terms analogous to Stark and Lamb shifts are neglected. If more than one degree of freedom of the system is coupled to the bath then the coupling term in Eq. (2) and dissipative terms (γ and D terms) in Eq. (3) should appropriately include additional similar contributions [see Eq. (14)].

The first term in Eq. (3) corresponds to the dynamical motion of the system that generates Liouville flow and the second term denotes the loss of energy from the system to the reservoir, while the last term indicates the diffusion of fluctuations of the reservoir into the system of interest. The terms containing γ arise due to the interaction of the system with the surroundings.

We note that Eq. (3) is a popular form of the operator master equation (as derived by Louisell[2]) which is widely used in quantum optics. The equation has also been applied earlier by Dittrich and Graham[7] in the treatment of dissipative standard map and the related problems of chaotic dynamics by others.[8, 16] The Eq. (3) is also general in the sense that we need not ascribe any notion of regularity or chaoticity in describing the motion governed by the Hamiltonian system (H_0). The correlation between different forms of operator master equation has been reviewed in ref. 5. All of them, however, are not well-suited for numerical simulation. Equation (3) suits this purpose well. We shall return to this issue in Section IV to verify the theoretical propositions. We note, in passing, that Eq. (3) is based on rotating wave approximation and Born–Markov approximation. The latter approximation restricts its validity to weak damping limit only.

B. Semiclassical Theory

Our next task is to go over from a full quantum operator problem to an equivalent *c*-number problem described by the Hamiltonian (2). To this end we consider the quasi-classical distribution function $W(\{q_i\}, \{p_i\}, t)$ of Wigner[28]. The time evolution of this phase space function of the dynamical system characterized by the c-number variables $\{q_i, p_i\}$ is based on two considerations: First, one takes into account of the usual dynamical evolution under the influence of potential V as defined in (1). The second is the dissipative evolution of the system when it is coupled to the harmonic oscillator bath described by Eq. (2). The former is essentially rewriting Schrödinger equation in a quasi-classical langauge and has nothing to do with the latter. Thus we write

$$\left(\frac{dW}{dt}\right)=\left(\frac{\partial W}{\partial t}\right)_{\text{dynamical}}+\left(\frac{\partial W}{\partial t}\right)_{\text{dissipative}}$$

While the dynamical evolution is governed by Wigner equation,[28]

$$\begin{aligned}\left(\frac{\partial W}{\partial t}\right)_{\text{dynamical}} &= \sum_{i=1}^{N}\left[-\frac{p_i}{m_i}\frac{\partial W}{\partial q_i}+\left(\frac{\partial V}{\partial q_i}\right)\frac{\partial W}{\partial p_i}\right]\\ &\quad+\sum_{n_1+n_3+\cdots+n_N \text{ is odd and } >1}\left(\frac{\partial^{n_1+\cdots n_N}V}{\partial q_1^{n_1}\cdots\partial q_N^{n_N}}\right)\frac{(\hbar/2i)^{n_1+\cdots+n_N-1}}{n_1!\cdots n_N!}\\ &\quad\times\frac{\partial^{n_1+\cdots+N_N}}{\partial p_1^{n_1}\cdots\partial p_N^{n_N}}W\end{aligned}$$

the form of $(\partial W/\partial t)_{\text{dissipative}}$ is due to Caldeira and Leggett[5] as given by [when one of the system degrees of freedom is coupled to the reservoir as expressed in Hamiltonian (2); see the dissipative part of Eq. (5.14) of ref. 5]

$$\left(\frac{\partial W}{\partial t}\right)_{\text{dissipative}}=2\gamma\frac{\partial}{\partial p}pW+D\frac{\partial^2 W}{\partial p^2}$$

where γ and D have the same significance as in Eq. (3). The first term in the last equation is a direct consequence of the existence of a γ-dependent term in the imaginary part of the exponent in the expression for the propagator for the density operator of Feynman and Vernon theory and has been shown[5] to be responsible for appearance of a damping force in the classical equation of motion for the Brownian particle to ensure quantum-classical correspondence.

The total dynamics is a superposion of two contributions provided by the last two equations and when written elaborately we have;

$$\frac{dW}{dt} = \sum_{i=1}^{N}\left[-\frac{p_i}{m_i}\frac{\partial W}{\partial q_i} + \left(\frac{\partial V}{\partial q_i}\right)\frac{\partial W}{\partial p_i}\right]$$
$$+ \sum_{n_1+n_3+\cdots+n_N \text{ is odd and } >1} \left(\frac{\partial^{n_1+\cdots n_N} V}{\partial q_1^{n_1}\cdots\partial q_N^{n_N}}\right)\frac{(\hbar/2i)_1^n+\cdots+n_N-1}{n_1!\cdots n_N!}$$
$$\times\frac{\partial^{n_1+\cdots+N_N}}{\partial p_1^{n_1}\cdots\partial p_N^{n_N}} W + 2\gamma\frac{\partial}{\partial p} pW + D\frac{\partial^2 W}{\partial p^2} \tag{4}$$

That the two contributions to the total evolution of the Wigner function in Eq. (4) act independently in the overall dynamics is an assumption. This assumption is also implicit in the operator master equation (3) and has been routinely used in nonlinear and quantum optics, in general. (Note that Eq. (5.14) of ref. 5 carries the same message for a single-degree-of-freedom system). Strictly speaking, the γ and D terms in Eqs. (3) and (4) are valid if the system operators [i.e., q and p in Eq. (2)] pertain to a harmonic oscillator. When the system is nonlinear, as in the present case (also in many nonlinear optical situations) the usual practice is to add the additional contribution $-i[H_{\text{non}}, \rho]$ to the master equation [in the language of Fokker–Planck description this commutator, in general, contributes higher (third or more) order derivatives of the distribution] and to assume that the dissipative terms remain unaffected by the addition of the commutator term, H_{non} being the nonlinear part of the Hamiltonian H_0. The validity of this assumption was examined[29] earlier by Haake *et al.* and also by us. It is now known that this assumption is quite satisfactory within the perview of weak damping and/high temperature limit.

The equation (4) is a full quantum mechanical equation. A simple version of the above equation for one-degree-of-freedom system was used earlier by Zurek and Paz[18] for studying some interesting aspects of quantum-classical correspondence in relation to decoherence. The primary reasons for choosing Eq. (4) as our starting point for semiclassical analysis are (i) the rotating wave approximation (RWA) in the system-reservoir coupling has not been made in deriving Eq. (4) (ii) Eq. (4) is also free from Born approximation (or weak-coupling approximation) ensuring that the theory is valid even in the strong damping limit. (iii) Eq. (4) reaches the correct classical limit when $\hbar \to 0$, when D becomes the thermal diffusion coefficient in the high temperature limit. Thus Eq. (4) is a good description in the semiclassical limit. Keeping in view of these remarks and the earlier discussion in Section IIA we observe that Eq. (3) and Eq. (4) describe same dynamics in weakly dissipative systems. We adopt Eq. (4) for our semi-classical analysis that follows and Eq. (3) for quantum numerical simulation in Section IV to verify the theoretical propositions of this analysis.

The first term in Eq. (4) is the usual Poisson bracket which generates the Liouville flow. Both the Poisson bracket and the higher derivative terms result from an expansion of the Moyal bracket on the basis of an analytic $V(q)$. The last two terms have the same significance as in Eq. (3). It is important to note that the failure of correspondence between classical and quantum dynamics is predominantly due to higher derivative terms which make their presence felt roughly beyond the Ehrenfest regime.

As a first step it is convenient to introduce the following scaling of c-numbers $\{q_i, p_i\}$ in analogy to van Kampen's Ω-expansion;

$$\begin{aligned} q_i &= q_i(t) + \hbar^{1/2}\mu_i \\ p_i &= p_i(t) + \hbar^{1/2}v_i \end{aligned} \tag{5}$$

where $\hbar$ is the associated smallness parameter for the present analysis. μ and v in Eq. (5) refer to quantum fluctuations in co-ordinate and momentum, respectively. $q(t)$ and $p(t)$ are the corresponding classical co-ordinate and momentum. The time evolution of the distribution function of the fluctuation variables obeys

$$\frac{\partial\phi(\{\mu_i\},\{v_i\},t)}{\partial t} = \sum_k\left[-\frac{v_k}{m_k}\frac{\partial\phi}{\partial\mu_k} + \mu_j\frac{\partial^2 V}{\partial q_j\,\partial q_k}\frac{\partial\phi}{\partial v_k}\right] + 2\gamma\frac{\partial}{\partial v}v\phi + \mathcal{O}(\hbar^{1/2}) \tag{6}$$

Although this equation does not involve any $\hbar$ explicitly, it describes the time evolution of probability density function $\phi(\{\mu_i\},\{v_i\},t)$ for the quantum noise variables $\{\mu_i, v_i\}$, since ϕ is the lowest order quantum correction to classical distribution function $W(q_i(t), p_i(t), t)$. Secondly, the quantum dynamics enters into the picture when we put the quantum constraint (8) on the initial density function $\phi(\{\mu_k\},\{v_k\},0)$

$$\phi(\{\mu_k\},\{v_k\},0) = \prod_{k=1}^{N}\frac{1}{4\sigma}\exp\left[-\frac{\mu_k^2}{2\sigma^2} - 2\sigma^2 v_k^2\right] \tag{7}$$

as

$$\langle(\Delta\mu_i)^2\rangle^{1/2}\langle(\Delta v_i)^2\rangle^{1/2}=\sigma\cdot\frac{1}{2\sigma}=\frac{1}{2} \tag{8}$$

where $\hbar=1$ is used.

We thus note that the initial density $\phi(\mu, v, 0)$ is not a δ-function but has an appropriate spread. This spread incorporates the quantum noise which gets amplified as the density ϕ evolves in time. It is thus a quantum (minimum uncertainty product) condition and a requirement imposed by quantum-classical correspondence. v in Eq. (6) refers to the specific degree of freedom of the system to which the reservoir is coupled to allow the exchange of energy between the system and the reservoir.

As a second step we put Eq. (6) in a more compact form by invoking the symplectic structure of the Hamiltonian dynamics. For this, we specify

$$z_i=\begin{cases} q_i & \text{for} \quad i=1,..., N \\ p_{i-N} & \text{for} \quad i=N+1,..., 2N \end{cases} \tag{9}$$

Defining I as

$$I=\begin{pmatrix} 0 & E \\ -E & 0 \end{pmatrix} \tag{10}$$

where E is an $N\otimes N$ unit matrix, one can write the Hamilton's equation

$$\dot{z}_i=\sum_j I_{ij}\frac{\partial H}{\partial z_j} \tag{11}$$

Again we introduce the scaling z_i as

$$z_i=z_i(t)+\hbar^{1/2}\eta_i \tag{12}$$

with

$$\begin{aligned} \eta_i &= \mu_i && \text{for} \quad i=1,..., N \\ &= v_{i-N} && \text{for} \quad i=N+1,..., 2N \end{aligned} \tag{13}$$

corresponding to quantum fluctuations in co-ordinates (μ_i) and momenta (v_i). We generalize Eq. (6) further to the extent that all the momentum components $(\eta_i, i = N+1,..., 2N)$ are coupled to the bath linearly. One obtains the equation of motion for quantum fluctuation distribution function

$$\frac{\partial \phi}{\partial t} = -\sum_{i,\, j} \left[J_{ij} \eta_i \frac{\partial \phi}{\partial \eta_j} - 2\gamma_j \frac{\partial}{\partial \eta_j} (\eta_j \phi) \right] \tag{14}$$

where we have assumed that

$$\gamma_j = 0 \qquad \text{for} \quad j = 1,..., N$$

$$\gamma_j = \gamma \qquad \text{for} \quad j = N+1,..., 2N$$

Here

$$J_{ij} = \sum_k I_{ik} \frac{\partial^2 H}{\partial z_k \, \partial z_j} \tag{15}$$

contains the second derivatives of the potential and is a function of classical dynamical variables $z_i(t)$, (i.e., $p_i(t)$ and $q_i(t)$).

For further treatment Eq. (14) may be rewritten in a more compact form as follows:

$$\frac{\partial \phi}{\partial t} = [-\mathbf{F}(t) \cdot \nabla + 2N\gamma] \, \phi \tag{16}$$

where

$$\mathbf{F}(t) = \underline{J}(t) \, \eta - 2\gamma \underline{K} \eta \tag{17}$$

∇ refers to differentiation with respect to the components of η and $\underline{K}$ is a $2N \otimes 2N$ matrix defined as

$$k_{ij} = 0 \qquad \text{for} \quad i \neq j$$

$$k_{ii} = 0 \qquad \text{for} \quad i = 1,..., N$$

$$k_{ii} = 1 \qquad \text{for} \quad i = N+1,..., 2N$$

$\underline{J}$, the jacobian matrix as defined in (15) is a function of classical dynamical variables $\{q_i(t), p_i(t)\}$. The crucial question of stability/instability of classical motion in Hamiltonian systems essentially rests on this jacobian, or curvature (or second derivative) of the potential. Traditionally the local linear stability analysis around the fixed points is based on the assumption[22, 23] of constant curvature. However, the true stability of motion is only determined by keeping the time dependence of $\underline{J}$ (implicitly through $\{q_i(t), p_i(t)\}$) matrix intact. Also there is little connection between the local stability and global chaos. In view of this it is necessary to take full account of the time dependence of the curvature of the potential $\underline{J}(t)$ along the trajectory itself. When the motion of the dynamical system is regular $\underline{J}(t)$ is highly correlated throughout the entire course of evolution. On the other hand for chaotic motion when the dynamical variables in $\underline{J}$ (i.e., $\{q_i(t), p_i(t)\}$) by virtue of the classical equation of motions for $q_i(t)$ and $p_i(t)$ [or in general $z_i(t)$ of Eq. (9)] behaves *stochastically* $\underline{J}(t)$ describes a stochastic process. The loss of correlation in chaotic dynamical systems thus rests on the decay of correlation of fluctuations of $\underline{J}(t)$. What follows subsequently is a stochastic description of classical chaos in terms of this correlation.

Ever since the early numerical study of Chirikov mapping[30] revealed that the motion of a phase space variable $\{q \text{ or } p\}$ can be characterized by a simple random walk diffusion equation, attempts have been made to describe chaos in terms of a stochastic description (Langevin and Fokker–Planck description has been widely employed). It has now been realized that deterministic maps can result in long time diffusional processes and methods have been developed to predict successfully the corresponding diffusion coefficients.[31] In a number of recent studies[11, 24, 25] we have shown that the fluctuation in the curvature of the potential is amenable to a stochastic description in terms of the theory of multiplicative noise. This allows us to realize a number of important results of nonequilibrium statistical mechanics, like Kubo relation[24] fluctuation-decoherence relation[25] etc. in chaotic dynamics of a few-degree-of-freedom system.

Another important point to be noted here is that we *do not* make any *a priori assumption about the nature of the stochastic process* ($\mathbf{J}(t)$). The special cases, such as, noise is Gaussian or δ-correlated, etc. have attracted so much attention in the literature that it is necessary to emphasize that we have not made any such approximation. The stochasticity of $\mathbf{F}(t)$ depends on $\underline{J}$ which is determined by the exact solution of the classical equation of motion (11). Equation (16) may therefore be regarded as a stochastic differential equation with multiplicative noise. For convenience $\mathbf{F}(t)\cdot\nabla$ can be partitioned (this partitioning will be clarified in more detail in the next section) into two parts; a constant part $\mathbf{F}_0\cdot\nabla$ and a fluctuating part $\mathbf{F}_1(t)\cdot\nabla$. Thus we write

$$\mathbf{F}\cdot\nabla = \mathbf{F}_0\cdot\nabla + \mathbf{F}_1\cdot\nabla \tag{18}$$

We now come to the third step. Making use of one of the main results for the theory of linear equation of the form (16) with multiplicative noise, we derive an average equation for ϕ as given by (for details, we refer to[26, 27]);

$$\frac{\partial\langle\phi\rangle}{\partial t}=\Big\{-\mathbf{F}_0\cdot\nabla+2N\gamma-\langle\mathbf{F}_1\cdot\nabla\rangle$$
$$+\int_0^\infty d\tau\langle\langle\mathbf{F}_1(t)\cdot\nabla\exp(-\tau[\mathbf{F}_0\cdot\nabla+2N\gamma])\,\mathbf{F}_1(t-\tau)\cdot\nabla\rangle\rangle$$
$$\times\exp(\tau[\mathbf{F}_0\cdot\nabla+2N\gamma])\Big\}\langle\phi\rangle \tag{19}$$

where $\langle\langle\cdots\rangle\rangle$ implies $\langle\langle q_iq_j\rangle\rangle=\langle q_iq_j\rangle-\langle q_i\rangle\langle q_j\rangle$. The operator $\exp(-\tau\mathbf{F}_0\cdot\nabla)$ provides the solution of the equation

$$\frac{\partial f(\eta,t)}{\partial t}=-\mathbf{F}_0\cdot\nabla f(\eta,t) \tag{20}$$

(where f signifies the "unperturbed" part of ϕ) which can be found explicitly in terms of characteristic curves. The equation

$$\dot{\eta}=\mathbf{F}_0(\eta) \tag{21}$$

for fixed t determines a unperturbed mapping from $\eta(\tau=0)$ to $\eta(\tau)$, i.e., $\eta\to\eta^\tau$ with inverse $(\eta^\tau)^{-\tau}=\eta$. The solution of (20) is

$$f(\eta,t)=f(\eta^{-t},0)\left|\frac{d\eta^{-\tau}}{d\eta}\right|=\exp[-t\mathbf{F}_0\cdot\nabla]\,f(\eta,0) \tag{22}$$

$|d\eta^{-t}/d\eta|$ being a Jacobian determinant. The effect of $\exp(-t\mathbf{F}_0\cdot\nabla)$ on $f(\eta)$ is as follows

$$\exp(-t\mathbf{F}_0\cdot\nabla)\,f(\eta,0)=f(\eta^{-t},0)\left|\frac{d\eta^{-t}}{d\eta}\right| \tag{23}$$

When this simplification is used in Eq. (19) we obtain

$$\frac{\partial\langle\phi\rangle}{\partial t}=\Big\{-\mathbf{F}_0\cdot\nabla+2N\gamma-\langle\mathbf{F}_1\cdot\nabla\rangle+\int_0^\infty d\tau\left|\frac{d\eta^{-\tau}}{d\eta}\right|$$
$$\times\langle\langle\mathbf{F}_1(\eta,t)\cdot\nabla_\tau\mathbf{F}_1(\eta^{-\tau},t-\tau)\rangle\rangle\cdot\nabla_{-\tau}\left|\frac{d\eta}{d\eta^{-\tau}}\right|\Big\}\langle\phi\rangle \tag{24}$$

The above consideration is based on a second order expansion in $\alpha\tau_c$ (by van Kampen[26]), where α is the strength parameter required for bookkeeping the order of the perturbation fluctuation and τ_c is the correlation time of fluctuations in $\mathbf{F}_1(t)$ [in the derivation above we have put $\alpha = 1$]. The average $\langle \phi \rangle$ in Eq. (24) varies on a coarse-grained timescale which is much slower compared to the timescale set by the correlation time of fluctuation of $\mathbf{F}_1(t)$. Second, the derivation above neglects the effects of higher powers of $\hbar$ and thus the Eq. (24) is an effective semiclassical equation for quantum fluctuation distribution function. Since it contains second derivatives with respect to components of η, it has the form of a Fokker–Planck equation. Third, the theory discussed so far (Eq. (24)) is valid, in general, for N-degree-of-freedom systems.

We now adapt Eq. (24) to the classic paradigm of chaotic dynamics—the Henon–Heiles system.

III. THE DISSIPATIVE HENON–HEILES SYSTEM

A. The Fokker–Planck Equation

We consider the Henon–Heiles system which is kept in contact with the surroundings. The Hamiltanian of this system is given by

$$H_0 = \frac{p_1^2}{2} + \frac{p_2^2}{2} + V(q_1, q_2) \tag{25}$$

where $V(q_1, q_2) = \frac{1}{2}(q_1^2 + q_2^2 + 2q_1^2 q_2 - \frac{2}{3} q_2^3)$, is the potential energy of the two-degree-of-freedom system.

The classical equations of motion of the particle in presence of damping (at a rate γ) are

$$\begin{aligned} \dot{q}_i &= p_i \\ \dot{p}_i &= -\gamma p_i - \frac{\partial V(q_1, q_2)}{\partial q_i}, \qquad i = 1, 2 \end{aligned} \tag{26}$$

Note that in the above equation we have assumed for simplicity the value of dissipation rate same for both the degrees of freedom. The equations of motion for the quantum fluctuation variables η_1, η_2, η_3 and η_4 corresponding to q_1, q_2, p_1 and p_2, respectively, read as follows:

$$\frac{d}{dt}\begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \end{pmatrix} = \underline{J} \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \end{pmatrix} \tag{27}$$

Following the procedure as described in the last section $\underline{J}$ can be identified as

$$\underline{J}=\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1-\zeta_1(t) & \zeta_2(t) & 0 & 0 \\ \zeta_2(t) & -1+\zeta_1(t) & 0 & 0 \end{pmatrix} \tag{28}$$

Here $\zeta_1(t)$ and $\zeta_2(t)$ are given by

$$\begin{aligned} \zeta_1(t) &= 2q_2 \\ \zeta_2(t) &= -2q_1 \end{aligned} \tag{29}$$

Since both q_1, q_2 are determined by classical equations of motion (26), chaoticity of the trajectory imparts stochasticity in the dynamics of quantum fluctuations in Eq. (27). Thus, as elaborated in the last section, $\zeta(t)$ terms represent the stochastic part of the second derivative of the potential $V(q_1, q_2)$.

If one takes into consideration of the γ-term then $\mathbf{F}(t)$ in Eq. (18) can be written as,

$$\mathbf{F}=\mathbf{F}_0+\mathbf{F}_1(t) \tag{30}$$

where

$$\mathbf{F}_0=\begin{pmatrix} \eta_3 \\ \eta_4 \\ -\eta_1-2\gamma\eta_3 \\ -\eta_2-2\gamma\eta_4 \end{pmatrix} \tag{31}$$

and

$$\mathbf{F}_1(t)=\begin{pmatrix} 0 \\ 0 \\ -\zeta_1(t)\,\eta_1+\zeta_2(t)\,\eta_2 \\ \zeta_2(t)\,\eta_1+\zeta_1(t)\,\eta_2 \end{pmatrix} \tag{32}$$

The equations for the characteristic curves are

$$\begin{aligned}
\dot{\eta}_1 &= \eta_3 \\
\dot{\eta}_2 &= \eta_4 \\
\dot{\eta}_3 &= -\zeta_1(t)\,\eta_1 + \zeta_2(t)\,\eta_2 - 2\gamma\eta_3 - \eta_1 \\
\dot{\eta}_4 &= \zeta_2(t)\,\eta_1 + \zeta_1(t)\,\eta_2 - 2\gamma\eta_4 - \eta_2
\end{aligned} \tag{33}$$

Equation (33) describes the dynamics of quantum fluctuations in presence of dissipation. The mapping $\eta \to \eta^t$ can be found by solving the unperturbed version of Eq. (33) (i.e., the ζ terms are omitted) for discrete small steps of τ (which is consistent with the requirement that the correlation time is short and finite) and is given by [we refer to van Kampen[26] for details of treatment of multiplicative stochastic noise in Eq. (33)]

$$\begin{aligned}
\eta_1^{-\tau} &= -\tau\eta_3 + \eta_1 \\
\eta_2^{-\tau} &= -\tau\eta_4 + \eta_2 \\
\eta_3^{-\tau} &= \frac{\eta_1}{2\gamma}\,(e^{2\gamma\tau} - 1) + \eta_3 e^{2\gamma\tau} \\
\eta_4^{-\tau} &= \frac{\eta_2}{2\gamma}\,(e^{2\gamma\tau} - 1) + \eta_4 e^{-2\gamma\tau}
\end{aligned} \tag{34}$$

The Jacobian determinant of the transformation reads as

$$\left| \frac{d\eta^{-\tau}}{d\eta} \right| \simeq e^{4\gamma\tau} \tag{35}$$

where the terms of the order of τ^2 are neglected. This is well within the error bound $(\alpha^2\tau_c)$ as shown by van Kampen[26] and does not incorporate additional error in the analysis.

Also note that

$$\left| \frac{d\eta}{d\eta^{-\tau}} \right| \simeq e^{-4\gamma\tau} \tag{36}$$

Making use of the mapping transformations $\eta \to \eta^\tau$ (Eq. (34)) one calculates the first and second derivative terms in Eq. (24) [For details we refer to ref. 26]. The master equation (24) for the Henon–Heiles system can then be written down. This is

$$\frac{\partial\langle\phi\rangle}{\partial t}=\Big[-\eta_3\frac{\partial}{\partial\eta_1}-\eta_4\frac{\partial}{\partial\eta_2}+\{\eta_1+2\gamma\eta_3-(C_3\eta_1-B_3\eta_2+A_3\eta_2$$
$$-B_3'\eta_1+A_3\eta_1+B_3'\eta_2+B_3\eta_1+C_3\eta_2)$$
$$-(\langle\zeta_2(t)\rangle\,\eta_2-\langle\zeta_1(t)\rangle\,\eta_1)\}\,\frac{\partial}{\partial\eta_3}$$
$$+\{\eta_2+2\gamma\eta_4-(\langle\zeta_2\rangle\,\eta_1+\langle\zeta_1\rangle\,\eta_2)+(B_3\eta_2-C_3\eta_1-A_3\eta_2-B_3'\eta_1$$
$$-A_3\eta_1-B_3'\eta_2+B_3\eta_1-C_3\eta_2)\}\,\frac{\partial}{\partial\eta_4}+4\gamma+E_1\frac{\partial^2}{\partial\eta_3\,\partial\eta_1}+E_2\frac{\partial^2}{\partial\eta_4\,\partial\eta_2}$$
$$+F_1\frac{\partial^2}{\partial\eta_3\,\partial\eta_2}+F_2\frac{\partial^2}{\partial\eta_4\,\partial\eta_1}+G\left(\frac{\partial^2}{\partial\eta_3^2}+\frac{\partial^2}{\partial\eta_3\,\partial\eta_4}\right)$$
$$+H\left(\frac{\partial^2}{\partial\eta_4\eta_3}+\frac{\partial^2}{\partial\eta_4^2}\right)\Big]\,\langle\phi\rangle \tag{37}$$

where

$$E_1=A_4\eta_2^2+C_4\eta_1^2-\eta_1\eta_2(B_4'+B_4)$$
$$E_2=A_4\eta_1^2+\eta_1\eta_2(B_4+B_4')+C_4\eta_2^2$$
$$F_1=\eta_1\eta_2(A_4-C_4)+B_4\eta_2^2-B_4'\eta_1^2$$
$$F_2=\eta_1\eta_2(A_4-C_4)-B_4\eta_1^2+B_4'\eta_2^2$$
$$G=\eta_2^2(A_2+B_2)+\eta_1^2(C_2-B_2')+\eta_1\eta_2(A_2-C_2-B_2'-B_2)$$
$$+\eta_1\eta_4(B_3'+C_3)+\eta_2\eta_3(B_3-A_3)+\eta_1\eta_3(B_3'-C_3)-\eta_2\eta_4(A_3+B_3)$$
$$H=\eta_2^2(B_2'+C_2)+\eta_1^2(A_2-B_2)+\eta_1\eta_2(A_2-C_2+B_2+B_2')$$
$$-\eta_1\eta_4(A_3+B_3)+\eta_1\eta_3(B_3-A_3)-\eta_2\eta_4(B_3'-C_3)$$
$$+\eta_2\eta_3(C_3-B_3') \tag{38}$$

and

$$\left.\begin{aligned}
A_2 &= \int_0^\infty \langle\!\langle \zeta_2(t)\, \zeta_2(t-\tau) \rangle\!\rangle\, e^{-2\gamma\tau}\, d\tau \\
B'_2 &= \int_0^\infty \langle\!\langle \zeta_1(t)\, \zeta_2(t-\tau) \rangle\!\rangle\, e^{-2\gamma\tau}\, d\tau \\
A_3 &= \int_0^\infty \langle\!\langle \zeta_2(t)\, \zeta_2(t-\tau) \rangle\!\rangle\, e^{-2\gamma\tau}\tau\, d\tau \\
B'_3 &= \int_0^\infty \langle\!\langle \zeta_1(t)\, \zeta_2(t-\tau) \rangle\!\rangle\, e^{-2\gamma\tau}\tau\, d\tau \\
A_4 &= \int_0^\infty \langle\!\langle \zeta_2(t)\, \zeta_2(t-\tau) \rangle\!\rangle\, \tau\, d\tau \\
B'_4 &= \int_0^\infty \langle\!\langle \zeta_1(t)\, \zeta_2(t-\tau) \rangle\!\rangle\, \tau\, d\tau \\
B_2 &= \int_0^\infty \langle\!\langle \zeta_2(t)\, \zeta_1(t-\tau) \rangle\!\rangle\, e^{-2\gamma\tau}\, d\tau \\
C_2 &= \int_0^\infty \langle\!\langle \zeta_1(t)\, \zeta_1(t-\tau) \rangle\!\rangle\, e^{-2\gamma\tau}\, d\tau \\
B_3 &= \int_0^\infty \langle\!\langle \zeta_2(t)\, \zeta_1(t-\tau) \rangle\!\rangle\, e^{-2\gamma\tau}\tau\, d\tau \\
C_3 &= \int_0^\infty \langle\!\langle \zeta_1(t)\, \zeta_1(t-\tau) \rangle\!\rangle\, e^{-2\gamma\tau}\tau\, d\tau \\
B_4 &= \int_0^\infty \langle\!\langle \zeta_2(t)\, \zeta_1(t-\tau) \rangle\!\rangle\, \tau\, d\tau \\
C_4 &= \int_0^\infty \langle\!\langle \zeta_1(t)\, \zeta_1(t-\tau) \rangle\!\rangle\, \tau\, d\tau
\end{aligned}\right\} \qquad (39)$$

The above equation (37) is a Fokker–Planck equation for probability distribution of quantum fluctuations for the dissipative Henon–Heiles system. It is evident that stochastic averaging over classical chaos leads to the average equation and the correlation functions contained in $A_2 \cdots C_4$. The correlation of fluctuations of curvature of the classical potential thus determines the drift and diffusion terms of the Fokker–Planck equation.

It must be emphasized that this fluctuation has nothing to do with the stochasticity inherent in the system-heat bath model governed by Hamiltonian (2). We also point out that since the very notion of stochastic process in describing the curvature of the potential results in the diffusion terms, the stochastification imparts a kind of irreversibility in the evolution governed by the Fokker–Planck equation (37). The origin of this irreversibility is classical chaos and not due to any external influence. This is characteristic of the nonlinear system, itself.

B. The Solution of Fokker–Planck Equation

The appearance of the variables η_1, η_2, η_3 and η_4 in the diffusion terms precludes the possibility of an exact solution of Eq. (37). One thus takes resort to *weak noise approximation* (this is consistent with assumption that fluctuations are not too large) scheme. The diffusion terms (given in the Appendix) are thus assumed to be constant.

The resulting Fokker–Planck equation can be transformed to the following simple form

$$\frac{\partial\langle\phi\rangle}{\partial t} = \left[\lambda u \frac{\partial}{\partial u} + A \frac{\partial^2}{\partial u^2} + 4\gamma\right]\langle\phi\rangle \tag{40}$$

where

$$u = a\eta_1 + b\eta_2 + c\eta_3 + \eta_4 \tag{41}$$

and the constants λ, A, a, b, and c are given in the Appendix.

We then search for the Green's function or conditional probability solution for the system at u at time t given that it had the value u' at $t = 0$. The initial condition which is required to bring forth quantum-classical correspondence is represented by

$$p(u, t = 0) = \frac{\varepsilon}{\pi} e^{-\varepsilon(u-u')^2} \tag{42}$$

This means that ε should be chosen in such a way that corresponds to the minimum uncertainty product of the initial wave packet. For notational convenience we have used

$$\langle\phi(u, t)\rangle = p(u, t) \tag{43}$$

We now look for a solution of the equation (40) of the form

$$p(u, t) \mid (u', 0) = e^{G(t)} \tag{44}$$

where

$$G(t) = -\frac{1}{\Gamma(t)}(u - \Omega(t))^2 + \ln v(t) \tag{45}$$

We are to see that, we can, by suitable choice of $\Omega(t)$, $\Gamma(t)$ and $v(t)$, solve Eq. (40) subject to the initial condition

$$p(u, 0) \mid (u', 0) = \frac{\varepsilon}{\pi} e^{-\varepsilon(u-u')^2} \tag{46}$$

Comparison of this with (44) with $G(0)$ shows that

$$\Gamma(0) = \frac{1}{\varepsilon}, \qquad \Omega(0) = u', \qquad v(0) = \frac{\varepsilon}{\pi} \tag{47}$$

If we put (44) in (40) and equate the coefficients of equal powers of u we obtain after some algebra the following set of equations

$$\frac{1}{\Gamma^2}\frac{d\Gamma}{dt} = -\frac{\gamma'}{\Gamma} + \frac{D_1}{\Gamma^2} \tag{48}$$

$$\frac{d\Omega}{dt} = -\lambda\Omega \tag{49}$$

and

$$\frac{1}{v}\frac{dv}{dt} = 4\gamma - \frac{D_1}{2\Gamma} \tag{50}$$

where

$$\begin{aligned} \gamma' &= 2\lambda \\ D_1 &= 4A \end{aligned} \tag{51}$$

The relevant solution of $\Gamma(t)$ for the present problem which satisfies the initial conditions above is given by

$$\Gamma(t) = \Gamma(0)\, e^{-\gamma' t} + \frac{D_1}{\gamma'}(1 - e^{-\gamma' t}) \tag{52}$$

It is important to note that the expansion of the wave packet is determined by $\Gamma(t)$ which is controlled by the two parameters, D_1 and γ' which by the virtue of Eqs. (51) and (40) can be identified as the "renormalized" diffusion and drift coefficients, respectively. The origin of this "renormalization" is essentially classical chaos since these coefficients are the complicated functions of the correlation function of the fluctuations of the curvature of the potential.

C. Results: Quantum Fluctuations, Expansion of Phase Space and Entropy

Having obtained $p(\eta_1, \eta_2, \eta_3, \eta_4)$ we are now in a position to determine the various theoretical quantities. We calculate the quantum fluctuations of position and momentum variables. Since the conditional probability p is given is given by Eq. (44), this together with (48)–(50) may be employed to calculate first and second moments. Thus we express

$$\langle \eta_1 \rangle = \frac{\iiiint_{-\infty}^{\infty} p(\eta_1, \eta_2, \eta_3, \eta_4, t \mid \eta_1', \eta_2', \eta_3', \eta_4', 0)\, \eta_1\, d\eta_1\, d\eta_2\, d\eta_3\, d\eta_4}{\iiiint_{-\infty}^{\infty} p(\eta_1, \eta_2, \eta_3, \eta_4, t \mid \eta_1', \eta_2', \eta_3'\eta_4', 0)\, d\eta_1\, d\eta_2\, d\eta_3\, d\eta_4} \tag{53}$$

in terms of conditional probability p. Explicit calculation yields

$$\langle \eta_1 \rangle = \frac{\Omega(t)}{a} \tag{54}$$

Similarly we obtain

$$\langle \eta_1^2 \rangle = \frac{1}{2a^2}\, \Gamma(t) + \frac{\Omega(t)^2}{a^2} \tag{55}$$

The conjugate variable to η_1 is η_3 whose average is given by

$$\langle \eta_3 \rangle = \frac{\Omega(t)}{c} \tag{56}$$

Similarly

$$\langle \eta_3^2 \rangle = \frac{1}{2c^2}\, \Gamma(t) + \frac{\Omega(t)^2}{c^2} \tag{57}$$

Therefore the uncertainty in coordinate $\Delta\eta_1$ and that in its conjugate momentum $\Delta\eta_3$ are obtained as follows;

$$\Delta\eta_1^2 = \langle \eta_1^2 \rangle - \langle \eta_1 \rangle^2 = \frac{1}{a^2}\left[\frac{\Gamma(t)}{2}\right] \tag{58}$$

$$\Delta\eta_3^2 = \langle \eta_3^2 \rangle - \langle \eta_3 \rangle^2 = \left[\frac{\Gamma(t)}{2}\right]\frac{1}{c^2} \tag{59}$$

where the relations (54)–(57) have been used. The uncertainty product $\Delta\eta_1\, \Delta\eta_3$ at any time is given by

$$\Delta\eta_1\, \Delta\eta_3 = \frac{1}{2\,|a|\, c}\,\Gamma(t) \tag{60}$$

where $\Gamma(t)$ is determined by Eq. (52) subject to initial conditions (47). This implies that we are to choose $\varepsilon = 1/|a|\, c$ to satisfy the minimum uncertainty product condition for $t=0$, for the wave packet [i.e., $\Delta\eta_1\, \Delta\eta_3 = \frac{1}{2}$].

We now discuss the following results:

(i) The relation (60) illustrates the evolution of quantum fluctuation as a function of time in terms of $\Gamma(t)$ which by the virtue of Eq. (52) is determined by the initial condition $\Gamma(0)$ [Eq. (47)] and the other two parameters D_1 and γ'. *The early expansion of quantum fluctuations* has been recognized *as a typical signature of classical chaos* on a generic quantum phenomenon.[24, 25] Note that D_1 [$=4A$, see Eq. (51)] is the diffusion coefficient that appeared in the Fokker–Planck Eq. (40) [this is not to be confused with the thermal diffusion coefficient D in Eq. (4) which arises due to the interaction with the surroundings] and γ' refers to the modified dissipation rate of the system in contact with the surroundings and is related to λ [by Eq. (51)] which is determined by Eq. (A13). The diffusion coefficient D_1 and modification of dissipation rate are due to the correlation of fluctuations of the curvature of the classical potential $\zeta_1(t)$ and $\zeta_2(t)$ through $A_2 \cdots C_4$ in Eqs. (39) and (A1). The origin of diffusion coefficient D_1 and the modification of γ thus have purely deterministic origin.

To analyze the growth of quantum fluctuations quantitatively [Eq. (60)] we first consider the dissipative classical chaotic motion governed by Eq. (26). We choose the initial conditions for energies $\frac{1}{8}$ and $\frac{1}{6}$. These energy values are wellknown in the context of classical Henon–Heiles Hamiltonian. It is important to note that even within the restricted domain of weak dissipation, the dissipative Henon–Heiles system approaches a manifold reduced dimensionality. The timescale over which this reduction takes place is determined essentially by the magnitude of the damping constant γ. This classical behaviour is illustrared in Figs. 1(a) and 2(a) for $\gamma = 0.001$ for the energies $\frac{1}{8}$ and $\frac{1}{6}$, respectively. Figs. 1(b) and 2(b) depict the corresponding Poincare maps for the conservative ($\gamma = 0.0$) Henon–Heiles system. It is thus apparent that even weak dissipation profoundly alters the characteristics of the stochastic process represented by the classical Hamiltonian chaos. The attractor clearly lies at the center. To calculate classical ensemble average of the quantities like $\langle \zeta(t) \rangle$ and $\langle\langle \zeta(t)\, \zeta(t-\tau) \rangle\rangle$, we carry out averaging over long time series for the given initial condition. The numerical procedure has been discussed earlier in ref. 24.

Following Eq. (60) we plot the variation of uncertainty product $[\Delta\eta_1\, \Delta\eta_3]$ ($\Delta\eta_1$ and $\Delta\eta_3$ are the quantum variances corresponding to position and momentum for one degree of freedom, respectively) as a function

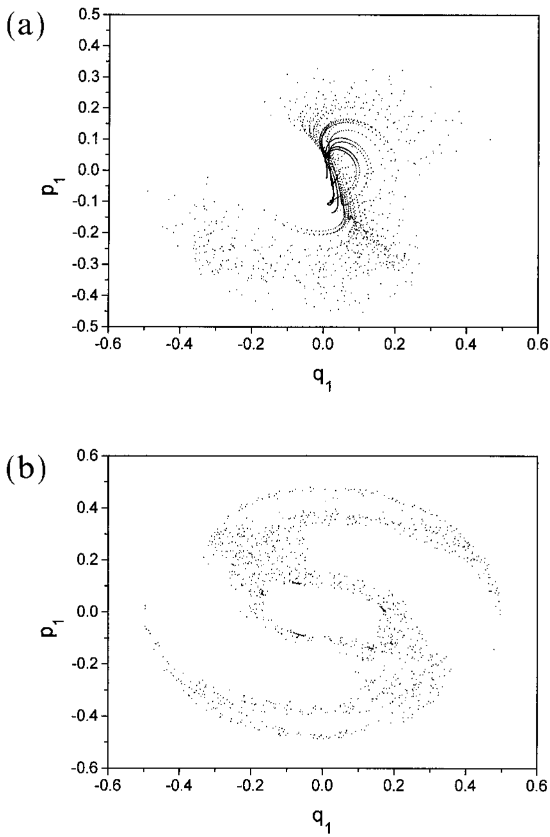

Fig. 1. (a) Plot of q_1 vs p_1 on the Poincaré surface of section for the Henon–Heiles system with damping constant $\gamma = 0.001$ and initial energy $E = \frac{1}{8}$. (b) Same as in (a) but for $\gamma = 0.0$.

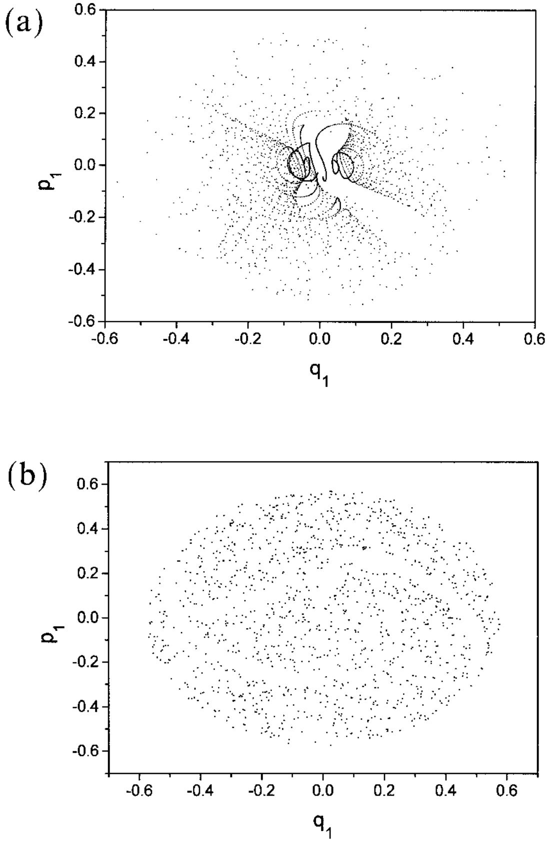

Fig. 2. (a) Same as in Fig. 1(a) but for $E=\frac{1}{6}$. (b) Same as in (a) but for $\gamma=0.0$.

of time for different values of energy corresponding to chaotic trajectories (damping rate $\gamma=0.001$) in Figs. 3 and 4. It has already been pointed out that the major input for the theoretical quantity are the chaotic diffusion coefficient D_1 and γ' which are further related to $A_2 \cdots C_4$, i.e., to classical correlation functions of the curvature of the potential. The theoretical curves are denoted in Figs. 3 and 4 by the dotted lines.

(ii) The relation (60) also shows that there exist *a critical limit to the expansion of phase space*. This limit is given by

$$\Delta\eta_1 \, \Delta\eta_3 |_{t \to \infty} = \frac{D_1}{2 \, |a| \, c\gamma'} \tag{61}$$

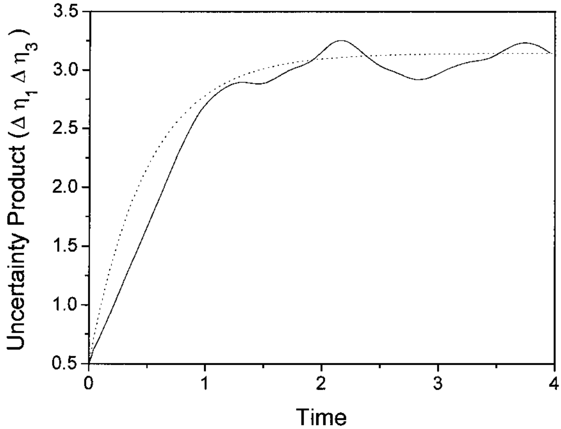

Fig. 3. Plot of uncertainty product ($\Delta\eta_1\,\Delta\eta_3$) with time for the system as in Fig. (1). The continuous line represents the numerical simulation of the master equation (fully quantum). The dotted line refers to semiclassical calculation (Eq. (60)). (Both units are arbitrary).

The existence of this critical width is a consequence of the competetion between chaotic diffusion, which attempts to expand the wave packet and dissipation γ which has the opposite tendency and this interplay ultimately leads to a compromised steady state.

At this juncture it is necessary to clarify the concept of steady state of the quantum dissipative system as applied here. The Henon–Heiles Hamiltonian is strongly nonlinear and so the notion of the thermodynamic

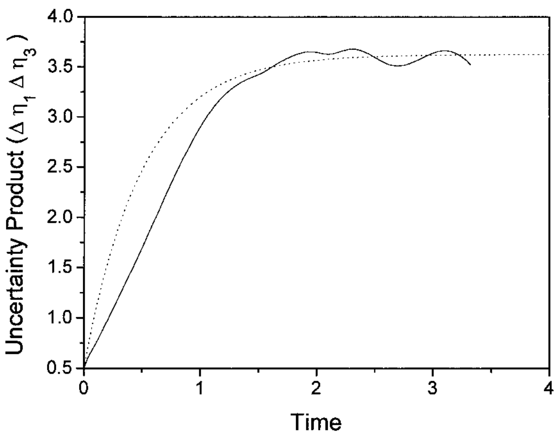

Fig. 4. Same as in Fig. 3 but for $E=\frac{1}{6}$.

equlibrium is inappropriate. Instead we mean a stationary state of the quantum system in the following sense. Here we are concerned with an asymptotic distribution of quantum noise variables η_i [$z_i = z_i(t) + \hbar^{1/2}\eta_i$, $z_i(t)$ being the classical position or momentum variable] in terms of the probability distribution function $\langle \phi(u, t) \rangle$ [$= p(u, t)$, u being the combination of quantum noise variables η_i (see Eq. (41)], rather than a distribution of $z_i(t)$s. Note that this function does not involve any classical contribution $z_i(t)$ directly. The classical chaotic fluctuation in $z_i(t)$s contribute to η_i via their classical correlation functions (in a, b, c of Eq. (41)). These correlations primarily determine the dynamics of η_i [see (49) and (54)] through λ where the role of γ is not the dominant one. This implies that although the classical motion of $z_i(t)$ settles down on an attractor approximately on a scale of, say, γ^{-1} as noted in Figs. 1(a) and 2(a), the quantum noise η_is approach the steady state very rapidly, i.e., in a few time units. Thus the present quantum steady state does not correspond to a settling down of classical motion on a attractor. Had we consider the asymptotic distribution of c-number variables z_i through the Wigner density function $W(z_i, t)$, then that would have correspond to an ideal quantum stationary state.

(iii) To make our analysis of irreversible evolution in presence of classical chaotic diffusion more quantitative, it is useful to calculate the entropy S of the Gaussian state by defining it[2] as

$$S = -p(t) \ln p(t) \tag{62}$$

where p is as defined by Eq. (44). In Fig. 5 we show the evolution of entropy due to quantum noise corresponding to the classical trajectories of the dissipative Henon–Heiles system for the energies $E = \frac{1}{6}$ and $\frac{1}{8}$ and $\gamma = 0.001$. At a very early stage the entropy change remains very small. It is then followed by a sharp increase and then finally tends to increase at a very slow rate. It is interesting to note that Zurek and Paz[18] advocated the efficacy of studying the evolution of entropy as a conseqence of interplay between Liouville dynamics and high temperature surrounding to examine the hall-mark of a nonintegrable system. Similar attempts had been made by us[11] earlier using Husimi distribution function to identify the different stages of quantum evolution.

Since the theory of stochastic fluctuations of the curvature of the potential rests on van Kampen's expansion in $\alpha\tau_c$ as emphasized earlier, care should be taken to calculate the integrals (39) over the correlation functions. To implement this numerically one considers the first fall of the correlation functions to adjust the cut off in time for numerical evalution of the integrals. This is a crucial requirement for the theory which should be appropriately taken care of in numerical calculation.

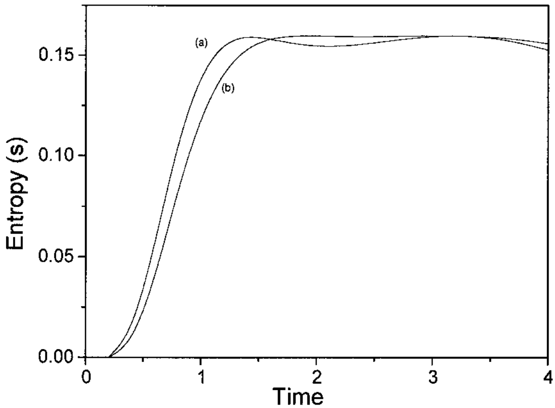

Fig. 5. Plot of evolution of entropy with time for damping constant $\gamma = 0.001$. (a) $E = \frac{1}{6}$ and (b) $E = \frac{1}{8}$.

We now point out a pertinent issue in the context of the nature of classical stochastic process considered here. It is wellknown that the Henon–Heiles model (without dissipation) is a typical KAM problem, i.e., it represents *soft chaos* and in principle never reaches the limit of fully developed *hard chaos*. This implies that, in a sense, classical noise has, in general, not very short correlation time. However the systematic procedure to deal with long correlation time when the nature of noise is rather unknown is relatively scarce. In principle, van Kampen's strategy as adopted here is applicable for consideration of higher order non-Markovian contributions. But such an extension is rather complicated both from analytical and numerical point of view. We therefore confine ourselves to the lowest order non-Markovian contribution to noise arising out of classical stochasticity and point out that such a description is not inappropriate in view of the short timescale over which the quantum fluctuations $\eta_i(t)$ determined by the correlations of the classical noise, persist.

IV. NUMERICAL SIMULATION OF THE QUANTUM OPERATOR MASTER EQUATION

For a full quantum-mechanical calculation to verify the basic theoretical propositions of semiclassical dynamics, we now return to Eq. (3). To solve the Eq. (3) for the Henon–Heiles system we choose two sets of basis vectors $\{|n_1\rangle\}$ and $\{|n_2\rangle\}$ of two different harmonic oscillators which satisfy $(\hat{p}_1^2/2m_1 + (1/2)\, m_1\omega_1^2\hat{q}_1^2)\, |n_1\rangle = [(n_1 + 1/2)\, \hbar\omega_1]\, |n_1\rangle$ and $(\hat{p}_2^2/2m_2 + (1/2)\, m_2\omega_2^2\hat{q}_2^2)\, |n_2\rangle = [(n_2 + 1/2)\, \hbar\omega_2]\, |n_2\rangle$. The frequencies ω_1 and ω_2

are arbitrarily adjusted to economize the size of the basis set. For the present purpose we choose $\omega_1 = 6.25$, $\omega_2 = 6.20$, $\hbar = 1$, and 35 basis vectors.

Quantum-classical correspondence is maintained through the construction of minimum uncertainty wave packets $|\alpha_{q_i, p_i}\rangle$ of Gaussian form in position and momentum representations having position $\langle q_i \rangle$ and average momentum $\langle p_i \rangle$ such that

$$\langle \alpha_{q_i, p_i} | n_i \rangle = [\exp(-0.5\, |\alpha_i|^2)]\, \frac{\alpha_i^n}{\sqrt{n_i!}} \tag{63}$$

where,

$$\alpha_i = \sqrt{m_i \omega_i / 2}\, [\langle q_i \rangle + (i/m_i \omega_i) \langle p_i \rangle], \qquad i = 1, 2$$

The quantum evolution is followed by locating the average positions and average momenta of the initial wave packets corresponding to the initial positions and momenta of two classically chaotic trajectories for the two energy values $\frac{1}{8}$ and $\frac{1}{6}$. Another important check for the numerical calculation is to keep the trace of the density matrix [Eq. (3)] equal to unity for the entire evolution. We have also checked that the result is robust against the variation of the size of the basis set. The numerical curves (solid lines) have been superimposed in Figs. 3 and 4 for the corresponding values of energy. It may be observed that the agreement between the theoretical and numerical curves is quite satisfactory. This justifies the validity of our semiclassical approach.

V. DISCUSSION ON THE APPROXIMATIONS, SUMMARY AND CONCLUSIONS

Based on a traditional scheme of system-reservoir model we have developed a theory of dissipative chaotic system. We make use of appropriate $\hbar$-scaling analogous to van Kampen's Ω-expansion, of equation for Wigner quasi-probability distribution functions which takes into account of thermal diffusion and dissipation due to the reservoir. We have shown that the semiclassical approximation leads us to an equation of motion for Wigner function for quantum noise which is governed by the dissipation due to reservoir and the second derivative of the classical potential, latter being a key-point in determining the stability of classical motion. Since chaoticity originates from the exponential loss of correlation of initially nearby trajectories this derivative behaves as a stochastic (deterministic) process. This stochastic process is amenable to a theoretical analysis (without imposing any a priori assumption about its nature) in terms of a treatment of stochastic differential equation with multiplicative noise. The resulting Fokker–Planck equation carries the information about the drift and diffusion coefficients which are expressible in terms of correlation functions of fluctuations of the curvature of the classical potential. As a prototypical example we have illustrated our analysis with the help of the Henon–Heiles Hamiltonian.

We now make a few remarks on the approximations involved in the present treatment and their validity.

(i) It must be emphasized that since the system-reservoir dissipative dynamics as governed by the operator master equation (3) is based on Born–Markov approoximation (the correlation time of the reservoir must be very short (Markov) for the interaction between the system and the reservoir to be sufficiently small (Born/weak coupling)), the underlying stochastic process due to the reservoir is *Markovian by construction.* On the other hand the stochasticity due to classical chaos as inherent in the fluctuations of the curvature of the potential is *non-Markovian* since we take account of short but finite correlation time of this fluctuations. The construction of the associated Fokker–Planck equation is based on a perturbative cumulant expansion in $\alpha\tau_c$, where τ_c is the correlation time of fluctuation of the curvature of the potential. The convergence of expansion as demonstrated by van Kampen[27] thus allows us to retain only upto second derivative terms and as such one need not go to third or higher order terms to describe the dynamics. While we note that there exist a vast body of literature in condensed matter and chemical physics dealing with finite time response of the reservoir which results in frequency dependence of friction coefficient γ, these and related aspects of dissipative dynamics are outside the scope of the present treatment. Our approach is similar to Graham *et al.*[7] and Milonni *et al.*[8] in this respect. Thus the short time regime, we believe, is mainly controlled by the curvature of the potential and the correlation of its fluctuations or in other words the short time dynamics is dominated by characteristic motion of the system itself. However, in the ultimate passage towards equilibrium the dissipation plays a prominent decisive role.

(ii) In the master equation (4), the classical stochasticity due to chaos and the quantum noise due to incoherent processes induced by the heat bath act simultaneously and influence one another. We have already noted that because of $\hbar$-scaling of this equation, one arrives at Eq. (6) in which the quantum noise term D due to surrounding does not appear in the lowest order. Thus it is because of strict semiclassical nature of our approach which is consistent with the consideration of dissipative contribution of $(\partial W/\partial t)_{\text{dissipative}}$ in Eq. (4) (valid for $kT > \hbar\omega$, because the propagator in the relevant integral form of the density operator master equation of Leggett and Caldeira [5.14 of ref. 5] has been approximated keeping in view of this inequality). However a simple calculation shows that the effect of this incoherent contribution makes its presence felt in the next order. The quantum noise due to surroundings becomes appreciable only at very low temperature.

(iii) We have already pointed out that Eq. (3) because of Born approximation is valid for weak damping case. We take care of this limitation by choosing small values of γ for carrying out numerical simulation of quantum master equation (3) and comparing our results with semiclassical analysis. The latter analysis based on Eq. (4) is free from Born approximation and is therefore valid for both weak and strong damping limits. For a comparison over the entire range of dissipation one needs simulation of other kinds of master equation which are free from weak coupling approximation. Unfortunately most of them are not well suited for numerical implementation.

We thus summarise the main conclusions of this study:

(i) The fluctuation of the second derivative of the potential due to classical chaos is amenable to a stochastic description when the correlation time of fluctuations is short but finite.

(ii) $\hbar$-scaling identifies an early stage of quantum evolution which is dominated by chaotic diffusion and dissipation but not by thermal diffusion.

(iii) The drift and diffusion terms of the Fokker–Planck equation are intrinsic characteristic of dynamical properties of the system since they depend crucially on the correlation of the fluctuations of the curvature of the potential. The dissipation is due to the coupling of the system to the external reservoir which causes irreversible evolution and is truely a many-body effect. On the other hand the chaotic diffusion imparts a kind of irreversibility in the evolution which has a strict deterministic origin and is characteristic of the nonlinear system itself.

(iv) The Fokker–Planck equation is reminiscent of Kramers' equation which describes the Brownian motion in phase space for thermally activated processes. The Fokker–Planck equation also assumes a generic form for two-degree-of-freedom systems, in general.

(v) Our results show how the initial quantum noise gets amplified by classical chaotic diffusion and then ultimately equilibriated with the passage of time under the influence of dissipation.

(vi) We establish that there exists a critical limit to the expansion of the phase space which is determined by chaotic diffusion and dissipation.

Henon–Heiles system is a classic Hamiltonian that illustrates deterministic stochasticity in two-degree-of-freedom systems. In view of its prototypical role played in earlier as well as in the present investigation, we hope that the conclusions drawn here will find qualititative and semiquantative applicability in other cases of dissipative two-degree-of freedom systems at the semiclassical level of description, in general.

APPENDIX A. THE TRANSFORMATION OF THE FOKKER–PLANCK EQUATION

The diffusion terms corresponding to (38) under weak noise-approximation are given by

$$E'_1 = A_4\eta_2^2(0) + C_4\eta_1^2(0) - \eta_1(0)\,\eta_2(0)(B'_4 + B_4)$$

$$E'_2 = A_4\eta_1^2(0) + \eta_1(0)\,\eta_2(0)(B_4 + B'_4) + C_4\eta_2^2(0)$$

$$F'_1 = \eta_1(0)\,\eta_2(0)(A_4 - C_4) + B_4\eta_2^2(0) - B'_4\eta_1^2(0)$$

$$F'_2 = \eta_1(0)\,\eta_2(0)(A_4 - C_4) - B_4\eta_1^2(0) + B'_4\eta_2^2(0)$$

$$\begin{aligned} G' &= \eta_2^2(0)(A_2 + B_2) + \eta_1^2(0)(C_2 - B'_2) + \eta_1(0)\,\eta_2(0)(A_2 - C_2 - B'_2 - B_2) \\ &\quad + \eta_1(0)\,\eta_4(0)(B'_3 + C_3) + \eta_2(0)\,\eta_3(0)(B_3 - A_3) + \eta_1(0)\,\eta_3(0)(B'_3 - C_3) \\ &\quad - \eta_2(0)\,\eta_4(0)(A_3 + B_3) \\ H' &= \eta_2^2(0)(B'_2 + C_2) + \eta_1^2(0)(A_2 - B_2) + \eta_1(0)\,\eta_2(0)(A_2 - C_2 + B_2 + B'_2) \\ &\quad - \eta_1(0)\,\eta_4(0)(A_3 + B_3) + \eta_1(0)\,\eta_3(0)(B_3 - A_3) - \eta_2(0)\,\eta_4(0)(B'_3 - C_3) \\ &\quad + \eta_2(0)\,\eta_3(0)(C_3 - B'_3) \end{aligned} \tag{A1}$$

Zeroes in $\eta_1(0)$, $\eta_2(0)$, $\eta_3(0)$ and $\eta_4(0)$ refer to their initial values corresponding to the initial preparation of the coherent wave packet which is centered around the classical position and momentum for the chaotic trajectory.

The Fokker–Planck equation (37) can then be written in a more compact form as follows;

$$\frac{\partial\langle\phi\rangle}{\partial t}=\left[-\eta_3\frac{\partial\langle\phi\rangle}{\partial\eta_1}-\eta_4\frac{\partial\langle\phi\rangle}{\partial\eta_2}+(\eta_1 k+\eta_2 l+2\gamma\eta_3)\frac{\partial\langle\phi\rangle}{\partial\eta_3}\right.$$
$$+(\eta_1 l+\eta_2 m+2\gamma\eta_4)\frac{\partial}{\partial\eta_4}\langle\phi\rangle+4\gamma\langle\phi\rangle+E'_1\frac{\partial^2\langle\phi\rangle}{\partial\eta_3\,\partial\eta_1}+E'_2\frac{\partial^2\langle\phi\rangle}{\partial\eta_4\,\partial\eta_2}$$
$$+F'_1\frac{\partial^2\langle\phi\rangle}{\partial\eta_3\,\partial\eta_2}+F'_2\frac{\partial^2\langle\phi\rangle}{\partial\eta_4\,\partial\eta_1}+G'\left(\frac{\partial^2}{\partial\eta_3^2}+\frac{\partial^2}{\partial\eta_3\partial\eta_4}\right)\langle\phi\rangle$$
$$\left.+H'\left(\frac{\partial^2}{\partial\eta_4\,\partial\eta_3}+\frac{\partial^2}{\partial\eta_4^2}\right)\right]\langle\phi\rangle \tag{A2}$$

where

$$\begin{aligned}k&=1-C_3+B'_3-B_3-A_3+\langle\zeta_1\rangle\\ m&=1-\langle\zeta_1\rangle+B_3-B'_3-A_3-C_3\\ l&=-B'_3-A_3-C_3+B_3-\langle\zeta_2\rangle\end{aligned} \tag{A3}$$

We now make the following transformation;

$$u=a\eta_1+b\eta_2+c\eta_3+\eta_4 \tag{A4}$$

where a, b and c are constants to be determined. Using this transformation we can write the Eq. (A2) as

$$\frac{\partial\langle\phi\rangle}{\partial t}=\left[\lambda u\frac{\partial}{\partial u}+A\frac{\partial^2}{\partial u^2}+4\gamma\right]\langle\phi\rangle \tag{A5}$$

where

$$A=E'_1ac+E'_2b+F'_1bc+F'_2a+G'(c^2+c)+H'(c+1) \tag{A6}$$

and

$$\lambda u=-\eta_3 a-\eta_4 b+\eta_1 ck+\eta_2 cl+2\gamma\eta_3 c+\eta_1 l+\eta_2 m+2\gamma\eta_4 \tag{A7}$$

Making use of Eq. (A4) in (A7) we obtain,

$$\begin{aligned}\lambda a&=ck+l\\ \lambda b&=cl+m\\ \lambda c&=-a+2\gamma c\\ \lambda&=2\gamma-b\end{aligned} \tag{A8}$$

The above relations can be used to obtain the following algebraic equation for λ

$$\lambda^4 + d_1\lambda^3 + d_2\lambda^2 + d_3\lambda + d = 0 \tag{A9}$$

where

$$\begin{aligned} d_1 &= -4\gamma \\ d_2 &= 4\gamma^2 + k + m \\ d_3 &= -2\gamma(k+m) \\ d &= mk - l^2 \end{aligned} \tag{A10}$$

We now seek for a perturbative solution of Eq. (A9). To this end let us first note that in the limit $\gamma \to 0$ Eq. (A9) reduces to a biqudratic form (since d_1 and d_3 vanishes) whose solution is given by

$$\lambda_0 = \pm\left[\frac{-d_2' \pm \sqrt{d_2'^2 - 4d}}{2}\right]^{1/2} \tag{A11}$$

where

$$d_2' = k + m \tag{A12}$$

The lowest order perturbative solution of the the Eq. (A9) is therefore given by

$$\lambda = \lambda_0\left[1 - \frac{d_1\lambda_0^2 + d_2 + 4\gamma^2\lambda_0}{4\lambda_0^4 + 3d_1\lambda_0^2 + 2d_2\lambda_0 + d_3}\right] \tag{A13}$$

For the present problem the positive real root of λ is allowed which satisfies the physical condition (the probability distribution function must vanish at $\pm\infty$). Now the values of the constants a, b and c which are used in Eq. (A4) can be calculated in terms of λ which is given by Eq. (A13) as follows

$$\begin{aligned} b &= 2\gamma - \lambda \\ c &= \frac{l}{\lambda(2\gamma - \lambda) - k} \\ a &= (2\gamma - \lambda)\, c \end{aligned} \tag{A14}$$

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