Quantization of the Stochastic Pump Model of Arnold Diffusion

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A semiclassical quantization of the stochastic pump model of Arnold diffusion is presented. The semiclassical model is found to be equivalent to a one-dimensional disordered wire, yielding localized states limiting the extent of diffusion. [S0031-9007(97)03422-4]

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Arnold diffusion [1] has long been considered a universal mechanism for global phase space flow in systems characterized as weakly chaotic [2–4]. It has also been a suspected source of instability in colliding beam storage rings [3–5] and magnetic traps [6], and its implications for the dynamics of Rydberg atoms [7] and of molecules [8] are under current investigation. A complete formal description of Arnold diffusion is still lacking, though upper bounds on rates have been established [9]. An approximate theory for classical Arnold diffusion is provided by the stochastic pump model [3,4,10], which has adequately predicted diffusion rates for a number of mappings. Despite these successes, it remains unclear how quantization changes the role of Arnold diffusion in weakly chaotic systems: Effects of quantization may be significant owing to the very slow rate of Arnold diffusion. Shuryak [11] presented dimensional arguments concerning the size of the classical actions required for quantum Arnold diffusion to be appreciable. In this Letter, we introduce a semiclassical quantization of the stochastic pump model of Arnold diffusion. We find the semiclassical model to be equivalent to a model describing single-particle transport in a one-dimensional (1D) disordered wire. Eigenstates of a disordered wire are localized [12], so that Arnold diffusion in this model is also limited by a finite localization length. The results presented here will also help us to understand how ergodicity arises in many-dimensional quantum systems that are classically weakly chaotic, suggesting a significant role for nonclassical "mechanisms" such as dynamical tunneling [13,14].

We examine the effect of quantization on Arnold diffusion in a system of coupled nonlinear oscillators. We consider a model where pairs of weakly coupled oscillators are coupled weakly to one another. The phase space structure of two weakly coupled oscillators contains regions of irregular motion separated by regular tori, guaranteed to exist by the Kolmogorov-Arnold-Moser (KAM) theorem [15]. Because chaotic motion is confined by the tori of the 2D system, no global instability is possible. In systems of higher dimension, however, chaotic regions are not separated from one another, and a globally connected web of irregular regions along which Arnold diffusion proceeds densely covers the energy surface [4]. Coupling one oscillator pair to a second pair provides the dimensionality required for Arnold diffusion, and is also a convenient model for the semiclassical quantization procedure described below. Each oscillator pair may in general be written as $H_p(\mathbf{J},\boldsymbol{\Theta}) = H_0(\mathbf{J}) + V(\mathbf{J},\boldsymbol{\Theta})$, and the small coupling expanded as $V(\mathbf{J},\boldsymbol{\Theta}) = \sum_{l,m} V_{l,m}(\mathbf{J}) e^{i\mathbf{n}\boldsymbol{\Theta}}$, where $\mathbf{n}$ is an integer vector. We can locally approximate $H_0(\mathbf{J})$ as $\sum_{i=2}^{2} (\omega_i J_i + \tilde{\omega}_i J_i^2)$ where the oscillator frequency is ω, and $\tilde{\omega}$ is the nonlinearity. We assume a low order resonance between the oscillators, $\omega_1/\omega_2 \approx s/r$, where r and s are small integers. The coupled oscillator pair Hamiltonian H_p can be rewritten as the sum of a resonance Hamiltonian $H_p^{(r)}$ and a second term containing both constants and the "fast" contributions $H_p^{(f)}$ [3]. The resonance Hamiltonian of the oscillator pair is $H_p^{(r)} = \frac{\tilde{\omega}_p}{2} I^2 - W_p \cos\Psi_p$, where $\tilde{\omega}_p = 2(r^2\tilde{\omega}_1 + s^2\tilde{\omega}_2)$; $\Psi_p = r\theta_1 - s\theta_2$; and $W_p = -2V_{r,-s}$. $H_p^{(r)}$ is also the Hamiltonian of a nonlinear pendulum, the dynamics of which is regular. Upon adding the fast terms, however, a narrow stochastic layer forms in the separatrix region, which plays the central role of driving Arnold diffusion [4] upon coupling the pair to additional oscillators. H_p is coupled to a second coupled pair $H_{p'}$, the latter characterized by the resonance $\omega_1'/\omega_2' \approx s'/r'$. Arnold diffusion results upon coupling the resonance Hamiltonians of each pair. Starting with the full Hamiltonian for the coupled pairs $\tilde{H} = H_p + H_{p'} + \tilde{V}$, $\tilde{V} = \sum_{\mathbf{n}} \tilde{V}_{\mathbf{n}}(\mathbf{J}) e^{i\mathbf{n}\boldsymbol{\Theta}}$, $\tilde{H}$ is transformed to slow angles Ψ_p and $\Psi_{p'}$; the largest coupling between the resonance Hamiltonians $H_p^{(r)}$ and $H_{p'}^{(r)}$ is $V_A \equiv \mu\cos(\Psi_p - \Psi_{p'})$, where $\mu = 2\tilde{V}_{r,-s,-r',s'}$. Transformed $\tilde{H}$ appears as $\tilde{H} = H_p^{(r)} + H_{p'}^{(r)} + V_A + H^{(f)}$, where $H^{(f)}$ contributes the fast terms that create thin stochastic zones in the phase space.

The general mechanism for Arnold diffusion in this oscillator system is captured by the stochastic pump model. Roughly, Arnold diffusion is driven by stochastic trajectories of one oscillator pair through V_A; regular trajectories lying in the resonance zone of H_p are "pumped" by irregular motion in the separatrix region of pair $H_{p'}$, driving diffusion along the resonance zone of H_p. The classical pump model approximates the coupling scheme as

$$H_A = H_p^{(r)}(I_p, \Psi_p) + \mu\cos(\Psi_p - \Psi_{p'}), \quad (1a)$$

$$H_S = H_{p'}^{(r)}(I_{p'}, \Psi_{p'}) + U_{p'}\cos(\Psi_{p'} - \phi_{p'}). \quad (1b)$$

$H_p^{(r)}$ is the pendulum Hamiltonian above. The coupling in (1b), where $U_{p'} = 2V_{-r',s'+1}$, is the term of $H_{p'}^{(f)}$ contributing most to the stochastic layer near the separatrix of $H_{p'}^{(r)}$; $\phi_{p'} = \Omega_{p'}t + \phi_0$, where $\Omega_{p'}$ is the driving frequency, taken to be the slower of ω_1' and ω_2'; the conjugate of $\phi_{p'}$ is $\overline{I}_{p'}$. The coupling $V_A = \mu\cos(\Psi_p - \Psi_{p'})$ between the pairs drives the Arnold diffusion. To make the stochastic pump Hamiltonian time-independent, the form of the classical pump model we quantize below, we add to $H_A + H_S$ the term $H_C = \Omega_{p'}\overline{I}_{p'} + \Psi_{p'}I_{p'}$, and define the time-independent stochastic pump Hamiltonian as $H = H_A + H_S + H_C$.

To quantize the stochastic pump model we adopt the semiclassical assumption [16] that the eigenstates of $\mathbf{H}_p$ or $\mathbf{H}_{p'}$ can be characterized as either regular or irregular. Irregular states correspond to phase space regions that are irregular; their density is primarily determined by the relative phase space density of the stochastic region around the separatrix of the resonance Hamiltonian. To have irregular states, the classical irregular region of an oscillator pair must be $>\hbar^2$. Following standard procedures given in Refs. [3,4], we obtain the size of the stochastic zone for (1b), setting the condition $\hbar < Ce^{-\pi Q_0/2}$, where $C = 8\pi U_{p'}\Omega_{p'}Q_0^2$; $Q_0 = \Omega_{p'}/\omega_{0p'}$ is the ratio of the high, driving frequency $\Omega_{p'}$ of the pump oscillator pair producing the stochastic layer, to the low, resonant frequency $\omega_{0p'} = (\tilde{\omega}_{p'}W_{p'})^{1/2}$ of the same pair; and $U_{p'}$ is the amplitude of the driving term in (1b). Within this framework we can write the Hamiltonian for the coupled oscillator system in a product basis of states that are either regular-regular, irregular-irregular, or regular-irregular. The latter is the subspace in which Arnold diffusion occurs. Irregular states are modeled by the Gaussian orthogonal ensemble (GOE) [17]. The stochastic pump Hamiltonian $H = H_A + H_S + H_C$ is quantized by coupling irregular states at those pumped sites, the regular states of $\mathbf{H}_p^{(r)}$, that are nearest-neighbor in action. The stochastic pump Hamiltonian $\mathbf{H}$ is written in the basis of the eigenstates of $\mathbf{H}_0 = \mathbf{H} - \mathbf{V}_A$. $\mathbf{H}_0$ contains the energy levels of a block-diagonal matrix, each block α being the same member of the GOE, providing the irregular states; plus the diagonal matrix $E_\alpha\mathbf{1}$, where E_α is the energy of the αth pumped level. The pumped levels are obtained from the Mathieu equation for the nonlinear resonance. For librational levels, we can approximate E_α as $\hbar\omega_{0p}\alpha + \hbar^2\tilde{\omega}_{0p}\alpha^2$, where $\omega_{0p} \approx (\tilde{\omega}_p W_p)^{1/2}$ is the local frequency and $\tilde{\omega}_{0p}$ the local nonlinearity. Rotational levels approach $E_\alpha = \hbar^2\tilde{\omega}_p\alpha^2$ as E_α surpasses the separatrix energy W_p, and we assume only rotational levels of the same symmetry couple.

The size of the elements of $\mathbf{V}_A$ are determined from a semiclassical relation between off-diagonal matrix elements of an operator, and the Fourier transform of its classical autocorrelation function [18]. The variance σ_v^2 of the elements of $\mathbf{V}_A$ depends on the energies of the states they couple; σ_v is very small when the energy difference is greater than $O(\hbar)$ [18]. For states close in energy, σ_v^2 appears in terms of the time integral of the autocorrelation function of V_A as

$$\sigma_v^2 \approx \hbar^{-1}\int dt\,\langle\delta V_A(t)\cdot\delta V_A(0)\rangle/4\pi\rho_s = \hbar^{-1}D_I/4\pi\rho_s\,, \tag{2}$$

where ρ_s is the density of irregular states given below. The second equality relates $\int dt\,\langle\delta V_A(t)\cdot\delta V_A(0)\rangle$ to the diffusion coefficient for the action I. This result is seen upon time integrating $\dot{I} = -\omega_p\sin\Psi_p + \mu\sin(\Psi_p - \Psi_{p'})$, where only the second term contributes over long times. The mean square displacement in I is then obtained from the time integration of $\mu\sin(\Psi_p - \Psi_{p'})$, which when $(I_{p'}, \Psi_{p'})$ execute motion in the irregular separatrix region is in the form of a Melnikov-Arnold integral. Similar calculations that have been carried out in Refs. [4,10] yield an expression for D_I with the same Melnikov-Arnold integral. Starting from the time integration of $V_A = \mu\cos(\Psi_p - \Psi_{p'})$, we see precisely that $D_I = \int dt\,\langle\delta V_A(t)\cdot\delta V_A(0)\rangle$. Following the analysis of Ref. [10], we find the action diffusion coefficient for the pumped oscillator pair to be

$$D_I \approx [16\pi^2R^2\exp(-\pi R)]\mu^2\Omega_{p'}^{-1}. \tag{3}$$

The ratio of frequencies of pairs p and p' is $R = \omega_{0p}/\omega_{0p'}$; μ is the strength of coupling between the oscillator pairs. The density of states ρ_s coupled by V_A is the density of pump states. We determine first the size of the classical stochastic region for H_0 [4]; then ρ_s is obtained from the semiclassical Weyl relation

$$\rho_s \approx \hbar^{-2}8\pi\Omega_{p'}^{-2}U_{p'}Q_0^3\exp(-\pi Q_0/2)\,. \tag{4}$$

The classical phase space density of the stochastic region is largely unaffected by the small coupling V_A [10].

The matrix model introduced to quantize the stochastic pump model is reminiscent of a 1D wire. Since the pump energies at all the sites along the wire are energy levels of a member of the GOE, and shifted from site to site, it is reasonable to assume the energies at each site are random and nearly independent, coupled by the random elements of $\mathbf{V}_A$. With this decorrelation assumption, it is apparent that our model is equivalent to a 1D disordered wire. The eigenstates of a disordered wire are localized. The localization length ξ_l has been determined by Efetov [12] using the nonlinear σ model to be $\xi_l = \pi\hbar^{-1}D_I\rho_s$. From (2), ξ_l for our model is $4\pi^2\sigma_v^2\rho_s^2$. Combining (3) and (4),

$$\xi_l \approx \hbar^{-3}A\exp(-\pi Q/2)\,, \tag{5}$$

where $A = 128\pi^4\mu^2U_{p'}R^2\omega_{0p'}^{-3}$, and $Q = Q_0 + 2R$. The extent of diffusion depends on how small the value of $\hbar$ is compared to $\exp(-\pi Q/2)$. To scale ξ_l with the actions of the coupled oscillators, we compare ξ_l with the width of the resonance zone of the pumped oscillator

pair, which is $L_r = \hbar^{-1} 4 (W_p/\tilde{\omega}_p)^{1/2}$. The criterion for $\xi_l \geq L_r$ is met when

$$\hbar \lesssim B \exp(-\pi Q/4), \tag{6}$$

where $B = 4\pi^2 \mu R \sqrt{2\omega_{0p} U_{p'}/\omega_{0p'}^3 W_p}$. The criterion of Eq. (6) is illustrated in Fig. 1, which shows the values of $\hbar$ and Q where diffusion a length at least the size of the resonance zone occurs. Notice that to guarantee irregular states in the semiclassical pump model we need to have $\hbar < C \exp(-\pi Q_0/2)$ as mentioned above. This is sometimes more restrictive than Eq. (6), though this depends on B and C, since typically $B < C$ due to small μ. Nevertheless, L_r serves only as a length scale with which to compare ξ_l, and we must bear in mind the overall localization of the eigenstates. Shuryak [11] presented dimensional arguments giving a criterion for widespread Arnold diffusion in quantum mechanical systems that has the form $\hbar \lesssim b \exp(-aQ_0)$. However, his dimensional arguments do not give the length along a resonance within which quantum Arnold diffusion is actually confined.

We turn now to some numerical studies of the semiclassical pump model. The aim is to check the extent to which the actual correlated matrix model of the stochastic pump is similar to that of the uncorrelated disordered wire used for the above estimates. We compare localization lengths of the random matrix model of the pump with those for the corresponding wire. In our numerics, $\mathbf{H}$ of the stochastic pump consists of a diagonal part $\mathbf{H}_0$, which is the solution to 80 blocks of dimension 24, each the same member of the GOE. The eigenvalues of each block labeled by α correspond to those of the pump states at each pumped site. The density of pump states at each site, ρ_s, is known from Wigner's semicircle law for the GOE. Taking the pumped states to be librational, the energy of the regular state at each site α is $E_\alpha = \hbar\omega_0\alpha + \hbar^2\tilde{\omega}_0\alpha^2$. The nonlinearity $\hbar^2\tilde{\omega}_0$ was set to values of $-10^{-6}S_s$ to $-10^{-4}S_s$, where $S_s = \rho_s^{-1}$; all values in this range yielded the same results. The elements of $\mathbf{V}_A$ couple the levels of one site to those of its neighboring sites; they are Gaussian random, and the same value is taken for elements coupling the same pair of irregular states between different pairs of coupled regular sites. We compare the average ξ_l of $\mathbf{H}$ at different $\Lambda \equiv \sigma_v^2 \rho_s^2$ and $\hbar\omega_0$ with that for the disordered wire at corresponding Λ. The wire is also modeled by 80 coupled GOE blocks of dimension 24, each block now a different member of the GOE. The results are plotted in Fig. 2. We see that ξ_l consistently follows the wire prediction of $\xi_l = 4\pi^2\Lambda$.

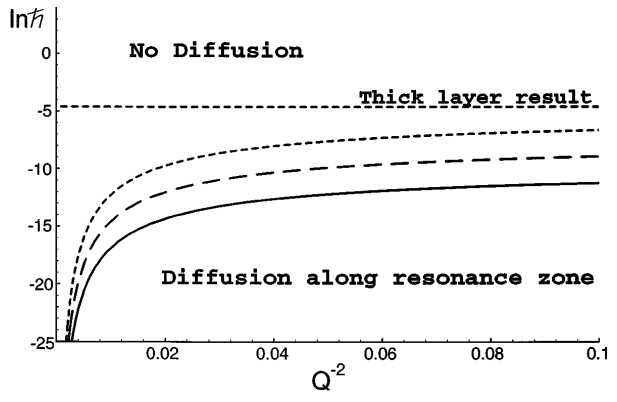

FIG. 1. Curves represent criterion for quantum Arnold diffusion a given length [Eq. (6)], in terms of $\hbar$ and Q^{-2}; Q^{-2} varies linearly with the coupling $U_{p'}$ between oscillators pumping diffusion. The coupling μ between the coupled oscillator pairs is 10^{-2} (short dashes), 10^{-3} (dashes), and 10^{-4} (line). The uppermost curve illustrates criterion for "thick layer" diffusion (see text).

We also compare results of ξ_l for a particular coupled oscillator system with ξ_l for the wire. We have analyzed numerically the Hamiltonian $H = H_{\rm qo} + H_m + V$, where $H_{\rm qo} = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{6}(bx^4 + b^{-1}y^4 - 2\lambda x^2 y^2)$; $H_m = \frac{1}{2}p_z^2 + D(1 - e^{-\alpha z})^2$; and $V = \gamma z x^2$. H_m can be written as $\omega_m I + \tilde{\omega}_m I^2$, where $\omega_m = \alpha\sqrt{2D}$ and $\tilde{\omega}_m = -\omega_m^2/2D$. Thousands of eigenstates of $H_{\rm qo}$ were previously analyzed and, to within a few percent, unambiguously assigned as either regular or irregular [19]. The product of the irregular states of $H_{\rm qo}$ and the (regular) states of H_m make up the basis of the pump model. We thus compute ξ_l for those H eigenstates that project primarily (>0.9) onto the irregular-regular (IR) subspace. In our computations $b = \pi/4$, $\omega_m = 1.2$, $\tilde{\omega}_m = 10^{-4}$, and $\lambda = 0.16$. For these parameters, we classified about 35% of the states in the range 501–580 as irregular, comparable to the estimate that ≈35% of the energy surface of the corresponding classical system is irregular [20]. We couple $H_{\rm qo}$ states 501–580 to 16 H_m sites, comprising the H basis. Elements of V are set by adjusting γ. For different Λ, determined numerically for H, we plot ξ_l in Fig. 2, where we see close agreement with the wire prediction. If we separate regular and

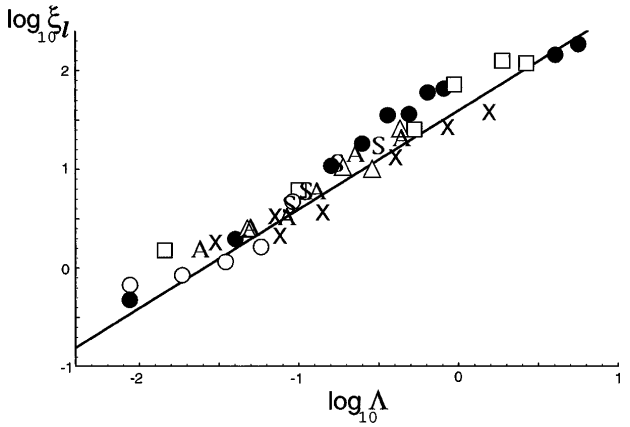

FIG. 2. Plotted are the average localization lengths at different $\Lambda \equiv \sigma_v^2 \rho_s^2$ obtained numerically for the random matrix models of the stochastic pump Hamiltonian; a coupled oscillator Hamiltonian (see text); and equivalent disordered wire. Filled circles are results for the wire model. Pump model results are plotted for $\hbar\omega_0 = 0.1$ (square); 0.3 (open circle); 0.7 (×); and 1.1 (triangle). Oscillators results include IR and RR states (A), and IR states only (S). The solid line is ξ_l predicted analytically for a disordered wire.

irregular states of $H_{\rm qo}$ and couple only irregular states of $H_{\rm qo}$ to H_m, we get similar results, also plotted in Fig. 2. Without separation, we find some eigenstates of H are a mixture of regular-regular (RR) and IR states. Still, the projection onto either IR or RR is >0.9 for about 99% of the eigenstates of H with the smallest γ plotted, and about 75% with the largest γ, so that any ambiguity from tunneling between IR and RR states is relatively small.

We finally consider the effect of additional oscillators in the general model. Introducing a third pair of coupled oscillators, which satisfy a resonance condition $\omega_1''/\omega_2'' \approx s''/r''$, where r'' and s'' are small integers, we couple the oscillator pairs by $\tilde{V} = \tilde{V}_{pp'} + \tilde{V}_{p'p''} + \tilde{V}_{pp''}$. The largest contribution to Arnold diffusion in this model arises from regular motion in the resonance zone of one pair driven by the irregular motion in any of the other pairs. The driving term in the pump model is then of the form $V_A = \mu_{pp'}\cos(\psi_p - \psi_{p'}) + \mu_{pp''}\cos(\psi_p - \psi_{p''})$. The quantization of this model again has the structure of a 1D disordered wire. The localization length is $\xi_l = \pi\hbar^{-1}D_I\rho_s$, where now calling $D_{I,pp'}$ the diffusion coefficient for pairs p and p', etc., we have $D_I = D_{I,pp'} + D_{I,pp''}$ and $\rho_s = \rho_{s,p'} + \rho_{s,p''}$. Assuming the D_I's and ρ_s's for all coupled pairs to be roughly the same, ξ_l over regular sites grows approximately as the square of the number of oscillator pairs in the system. The diffusion coefficients and level densities given by Eqs. (3) and (4) pertain to a stochastic region confined to the separatrix layer of the resonance zone. We must, however, bear in mind that the addition of oscillators increases the likelihood for intersection of primary resonances. Overlap or intersection of primary resonances profoundly alters the dynamics at the quantum level, and ultimately the localization, allowing energy flow to escape the 1D confines of a single resonance line of the Arnold web and be multidimensional and global [21]. In addition, classically, intersection of resonances among three or more oscillators generates chaotic dynamics in the vicinity of intersection [8]. Action diffusion again occurs along resonance zones that remain isolated, but is now driven by chaos occupying a much larger phase space fraction, regions of resonance intersection, than when all resonances are largely isolated, and only motion near the separatrix serves as a pump. Arnold diffusion driven by thick regions of strong chaos at resonance intersections has been termed "thick layer" diffusion [4]. The 3 oscillator model studied numerically could be said to be in this regime. The effect of resonance intersection on the quantized pump model is to dramatically increase ρ_s and D_I. The density of irregular states depends now on the region of resonance intersection, rather than the exponentially small stochastic layer. Thus $\xi_l \sim \hbar^{-1}D_I\rho_s$ varies as a polynomial in the small coupling ϵ between oscillators, rather than $e^{-K/\sqrt{\epsilon}}$, which over a given length greatly extends possible values of $\hbar$ and couplings for which quantum Arnold diffusion can proceed as illustrated in Fig. 1. Quantum thick layer Arnold diffusion appears in the nuclear motion of molecules. Perry *et al.*'s analysis of rotation-vibration coupling in ethanol [22], for instance, can be interpreted as quantum thick layer Arnold diffusion.

In conclusion, we have introduced a semiclassical quantization of the stochastic pump model of Arnold diffusion. We have argued that the semiclassical model is equivalent to a 1D disordered wire. Numerical results for the pump model support this correspondence. The states of the pump model are thus localized for any finite $\hbar$. The localization length is expressed in terms of $\hbar$ and classical properties of the model.

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