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DYNAMICAL STOCHASTICITY IN NONLINEAR QUANTUM SYSTEMS

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The properties of nonlinear quantum systems that are stochastic in the classical limit are investigated. It is shown for a definite model that for the quantum system, in contrast to the corresponding classical system, the Kolmogorov–Sinai entropy is zero, and the correlations are damped only as a power and not exponentially.

There has recently been a considerable growth of interest in the dynamics of nonlinear quantum systems [1-7] that are Kolmogorov systems [8, 9] in the classical limit ($\hbar = 0$). In the present paper, taking a simple model, we show that such quantum systems do not possess the typical properties of classical stochastic systems, namely, a nonvanishing Kolmogorov–Sinai entropy [10-11] and exponential damping of correlations.

We consider the model of a rotor in an external field with Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2J}\frac{\partial^2}{\partial\theta^2} + \tilde{k}(t)\cos\theta\delta_{\tilde{T}}(t), \tag{1}$$

where $\tilde{k}(t)$ is the parameter which characterizes the magnitude of the perturbation,

$$\delta_{\tilde{T}}(t) = \sum_{n=-\infty}^{\infty}\delta(t-n\tilde{T})$$

is a train of delta functions (jolts), J is the moment of inertia of the rotor, and θ is the angular variable. In what follows, J = 1.

The corresponding classical problem for $\tilde{k}$ = const was investigated in detail in [12], in which it was shown that for $\tilde{k}\tilde{T} \gg 1$ the rotor energy increases in accordance with the diffusion law

$$E(t) = \frac{\tilde{k}^2}{4}t + E(0). \tag{2}$$

Here and in what follows, t is the dimensionless time, measured by the number of jolts. For almost all initial conditions, except for small (when $\tilde{k}\tilde{T} \gg 1$) islands of stability, neighboring trajectories diverge exponentially: $d = d_0\exp(ht)$, where $d = \sqrt{(\tilde{T}\Delta p)^2 + (\Delta\theta)^2}$, and $h \approx \ln(\tilde{k}\tilde{T}/2)$ (for $\tilde{k}\tilde{T} > 4$) is the Kolmogorov–Sinai entropy [12].

To investigate the quantum system (1), we proceed from the equations for the Heisenberg operators, which after integration over the period $\tilde{T}$ go over into the operator mapping

$$\hat{p}_{t+1} = \hat{p}_t + \tilde{k}(t)\sin\hat{\theta}_t, \quad \hat{\theta}_{t+1} = \hat{\theta}_t + \tilde{T}\hat{p}_{t+1}, \tag{3}$$

where $\hat{p}_t$ and $\hat{\theta}_t$ are operators which satisfy the commutation relation $[\hat{p}_t, \hat{\theta}_t] = -i\hbar$. For $\hbar = 0$, (3) goes over into the standard mapping for a classical rotor [12].

It should be noted that in (3) the operator $\hat{\theta}$ corresponds to a continuous phase, which varies from $-\infty$ to ∞. In the case of a flat rotor, the operator $\hat{p}$ can be represented in the form $\hat{p} = -i\partial/\partial\theta$ [13]. The periodic phase φ, which varies in the interval from 0 to 2π, can be determined by means of the relation $\hat{\varphi} = \Phi(\hat{\theta})$, where $\Phi(x)$ is a periodic (with period 2π) discontinuous function, with $\Phi(x) = x$ for $0 \le x < 2\pi$ [13]. Since $\hat{\varphi}_t = U^+\Phi(\hat{\theta}_0)U = \Phi(\hat{\theta}_t)$ (U is the evolution operator (1)), for an arbitrary periodic function g (with period 2π) the relation $g(\hat{\varphi}_t) = g(\hat{\theta}_t)$ holds and therefore it is sufficient in what follows to investigate the

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properties of the operator $\hat{\theta}_t$, which uniquely determines $\hat{\varphi}_t$.

To analyze the mapping (3), we represent $\hat{p}_t$ and $\hat{\theta}_t$ in normal form with respect to the initial operators $\hat{p}_0$ and $\hat{\theta}_0$ (suppose, for example, all the $\hat{p}_0$ are on the right) after which it is a simple matter to obtain the projection of these operators onto the space of the initial states. Such a method of investigation in the quasiclassical approximation was used in [3].

It can be shown that for the operator mapping (3) one can obtain an exact normal form of $\hat{p}_t$ and $\hat{\theta}_t$. This makes it possible to show that in the quantum case the correlations decrease with the time not faster than a certain power of the time, in contrast to the exponential damping in a classical system, and the Kolmogorov–Sinai entropy of the quantum system is zero.

Using the well-known equation (see, for example, [14])

$$\exp(\hat{a}+\hat{b})=\exp(\hat{b}(e^c-1)/c)\exp(\hat{a}) \tag{4}$$

for operators with the commutation relation $[\hat{a}, \hat{b}]=c\hat{b}$, we obtain

$$\hat{p}_1=\hat{p}_0+\tilde{k}(0)\sin\hat{\theta}_0, \quad \hat{p}_2=\hat{p}_1+\Delta\hat{p}_2,$$

$$\Delta\hat{p}_2=\frac{\tilde{k}(1)}{2i}\left\{\sum_{m_0=-\infty}^{\infty}J_{m_0}(k_{1,0})\exp\left\{i\frac{T}{2}(m_0+1)\right\}\exp\{i(m_0+1)\hat{\theta}_0\}\exp\{i\hat{p}_0\tilde{T}\}-\text{c.c.}\right\}, \tag{5}$$

where $k_{1,0}=2k(0)\sin(T/2)$, $k(0)=\tilde{k}(0)/\hbar$, $T=\tilde{T}\hbar$, $J_{m_0}(k_{1,0})$ is a Bessel function and c.c. denotes the complex conjugate term. It follows from (3) and (5) that the normal form $\Delta\hat{p}_3=\tilde{k}(2)\sin\hat{\theta}_2$ with respect to $\hat{p}_1$ and $\hat{\theta}_1$ is obtained from $\Delta\hat{p}_2$ by the index substitution $1\to 2$, $0\to 1$. Applying (4), we obtain from it the normal form of $\Delta\hat{p}_3$ with respect to $\hat{p}_0$, $\hat{\theta}_0$. An arbitrary $\Delta\hat{p}_{t+1}=\tilde{k}(t)\sin\hat{\theta}_t$ is obtained from $\Delta\hat{p}_t$ recursively. Thus, if $\hat{p}_t$ and $\hat{\theta}_t$ are already represented in normal form, then

$$\hat{p}_{t+1}=\hat{p}_t+\Delta\hat{p}_{t+1}, \quad \hat{\theta}_{t+1}=\hat{\theta}_t+\tilde{T}\hat{p}_{t+1}, \quad \Delta\hat{p}_{t+1}=\frac{\tilde{k}(t)}{2i}\left\{\sum_{m_0,m_1,\ldots,m_{t-1}=-\infty}^{\infty}J_{m_0}(k_{1,t-1})J_{m_1}(k_{2,t-2})\ldots J_{m_{t-1}}(k_{t,0})\times\right. \tag{6}$$

$$\left.\exp(i\varphi_{m_0,\ldots,m_{t-1}})\exp(i\alpha_{m_0,\ldots,m_{t-1}}\hat{\theta}_0)\exp(i\beta_{m_0,\ldots,m_{t-1}}\tilde{T}\hat{p}_0)-\text{к. с.}\right\},$$

where

$$\varphi_{m_0}=\frac{T}{2}(1+m_0), \quad \alpha_{m_0}=m_0+1, \quad \beta_{m_0}=1, \quad \varphi_{m_0,\ldots,m_n}=\varphi_{m_0,\ldots,m_{n-1}}+\frac{T}{2}m_n(\alpha_{m_0,\ldots,m_{n-1}}+\beta_{m_0,\ldots,m_{n-1}})+\frac{T}{2}\alpha^2_{m_0,\ldots,m_{n-1}},$$

$$\alpha_{m_0,\ldots,m_n}=\alpha_{m_0,\ldots,m_{n-1}}+m_n, \quad \beta_{m_0,\ldots,m_n}=\alpha_{m_0,\ldots,m_{n-1}}+\beta_{m_0,\ldots,m_{n-1}} \quad k_{n,t}=2k(t)\sin\frac{T}{2}\beta_{m_0,\ldots,m_n}.$$

To investigate the obtained mapping, we project (6) onto the basis of initial states $\psi_n(\theta_0)=(2\pi)^{-1/2}e^{in\theta_0}$. Then (6) goes over into a c-number mapping (with $\hat{p}_0$ replaced by $\hbar n$), which can be regarded as a mapping describing the dynamics of some classical system for which the mean values of p_t and θ_t,

$$\langle p_t\rangle=\frac{1}{2\pi}\int_0^{2\pi}p_t(n,\theta_0)\,d\theta_0,$$

coincide with the quantum mean values and which in the limit $\hbar\to 0$ goes over into a classical system with standard mapping ((3) with $\hbar=0$). Thus, to understand the properties of the quantum system, we must study the classical system described by the mapping (6), where p_0 and θ_0 are c numbers. Note that the obtained mapping does not conserve the Jacobian $\mathcal{J}=\partial(p_t,\theta_t)/\partial(p_0,\theta_0)$ (for $\hbar=0$, $\mathcal{J}=1$), which oscillates with the time, which indicates the presence of "damping" with variable sign.

We consider the case when $k(t)=k=\text{const}$. In the classical case ($\hbar=0$), $m_0\sim kT$, $m_1\sim m_0kT\sim(kT)^3$, etc. Therefore, $\alpha_{m_0,\ldots,m_{t-1}}\sim(kT)^t$, $\partial\theta_t/\partial\theta_0\sim\alpha_{m_0,\ldots,m_{t-1}}\sim(kT)^t$ and neighboring trajectories diverge exponentially. For $\hbar\neq 0$ when $t<t_s$, we have

$$t_s\sim\ln(\tilde{k}/\hbar)/\ln(\tilde{k}\tilde{T}), \tag{7}$$

i.e., as long as $T\beta_{m_0,\ldots,m_{ts}}\ll 1$, the sine in the Bessel function in (6) can be replaced by its argument, and then, as before, we have local instability of neighboring trajectories. When $t>t_s$, we use the circumstance that in (6) $|m_n|\leqslant 2k$ (otherwise, $J_{m_n}(k)$ is exponentially small), and, therefore, $|\alpha_{m_0,\ldots,m_{t-1}}|\leqslant 2kt$, $|\beta_{m_0,\ldots,m_{t-1}}|\leqslant 2kt^2$. Then $d/d_0\sim(|\beta_{m_0,\ldots,m_t}|+|\alpha_{m_0,\ldots,m_{t-1}}|)\leqslant 2kt^2$ for $t>t_s$, and the entropy h decreases with the time in accordance

with the formula

$$h\sim(\ln k+2\ln t)/t. \tag{8}$$

Thus, for the system (1) the entropy is zero and, hence, (1) is not a Kolmogorov system, although for the corresponding classical system $h \approx \ln(kT/2) > 0$ $(kT > 4)$ [12]. Note that for $k(t) = k(0)t^{\alpha}$ the entropy also tends to zero in accordance with a law nearly the same as (8) (there is a different constant in front of $\ln t$). And it is only when $k(t) \sim \exp(\mu t)$ (this system is actually of no physical interest) that the entropy of the quantum system is nonzero: $h = \mu$.

We now consider the behavior of the different-time correlation functions in the quantum system (1): $R(t, n, q)=\frac{1}{2}\langle n|e^{-iq\hat{\theta}_0}e^{i\hat{\theta}_t}+e^{i\hat{\theta}_t}e^{-iq\hat{\theta}_0}|n\rangle$, where the mean value is taken with respect to the initial state $\psi_n(\theta_0)=(2\pi)^{-1/2}\exp(in\theta_0)$. From (6), we obtain an expression for $R(t, n, q)$ (k = const):

$$R(t, n, q)=\frac{1}{2}\sum_{m_0,\ldots,m_{t-1}} J_{m_0}(k_1)J_{m_1}(k_2)\ldots J_{m_{t-1}}(k_t)\exp(i\varphi_{m_0,\ldots,m_{t-1}})\times$$

$$\exp(i\beta_{m_0,\ldots,m_{t-1}}Tn)(1+\exp(-i\beta_{m_0,\ldots,m_{t-1}}Tq))\delta_{\alpha_{m_0,\ldots,m_{t-1}},q}. \tag{9}$$

For $t < t_s$, the quantum corrections in (9) can be ignored and the classical value of R used. Then $R(t, n, q)\sim e^{-\sigma t}$, where $\sigma\sim\frac{1}{2}\ln(kT)$ [3, 15]. At the time $t \sim t_s$ (7), the correlations reach the value $R(t_s, n, q)\sim 1/k^{1/2}$, and for the subsequent calculation of R it is necessary to use the exact expression (9), which presents considerable difficulties. We therefore restrict ourselves to a rough estimate and lower limit for $|R(t, n, q)|$.

For $t \gg t_s$ and almost all m_j $(j>t_s)$ $k_j\sim k$. Assuming also that φ and βT are distributed with equal probability in the interval $[0, 2\pi]$ (then

$$\sum_{m_j=-\infty}^{\infty} J_{m_j}(k)e^{i\varphi_{mj}}\approx 1)$$

we obtain $R(t, n, q)\sim R(t_s, n, q)\sim k^{-1/2}$, $t>t_s$. To find the maximal rate of decrease of $R(t, n, q)$, we use the condition of unitarity of the operator $e^{i\hat{\theta}_t}$ and the identity $\langle n|\exp(-i\hat{\theta}_t)\exp(i\hat{\theta}_t)|n\rangle\equiv 1$, from which we have

$$\exp(i\hat{\theta}_t)|n\rangle=\left(\sum_{m=-\infty}^{\infty}A_m^{(n)}e^{im\theta_0}\right)|n\rangle \text{ and } \sum_{m=-\infty}^{\infty}|A_m^{(n)}|^2=1.$$

But it follows from (6) (since $\alpha_{m_0,\ldots,m_{t-1}}\sim kt$), that the sum over m contains $m_{max} \sim kt$ terms ($A_m^{(n)}$ with $|m|>m_{max}$ are exponentially small). Assuming that all A_m with $|m| < m_{max}$ are of the same order (otherwise there is a q with $|q| < m_{max}$ for which the correlations will decrease slower than (10)), and using the exact equation $R(t, n, q)=\frac{1}{2}(A_q^{(n)}+A_q^{(n-q)})$, we obtain for $t \gg t_s$

$$|R(t, n, q)|\geqslant 1/\sqrt{kt}. \tag{10}$$

In the case $k(t) = kt^{\alpha}$, we must in (10) make the substitution $t\to t^{1+\alpha}/(1+\alpha)$.

Note that although the classical value of the correlation function will already differ from the quantum value after the time $t \sim t_s$ (in the comparison, we consider the quasiclassical region), the absolute value of the correlation function will be small, $R\sim\sqrt{\hbar/k}$, and therefore quantities that do not decrease in the classical case (for example, the rotor energy $E=\langle n|\frac{1}{2}\hat{p}_t^2|n\rangle$), will differ by a small amount $\sim(\hbar/k)^{1/2}$ during a time $t_0 \propto 1/\hbar$ (the number of correlation functions increases with the time as a power). A more accurate estimate for t_0 [7] gives ($\alpha \leq \frac{1}{2}$)

$$t_0\sim[(k/\hbar)^2(1-2\alpha)]^{1/(1-2\alpha)}. \tag{11}$$

It is interesting that for $\alpha > \frac{1}{2}$ the quantum corrections remain small at all times.

Finally, it should be noted that the reason for the power decrease of the correlations is the power growth of the number of θ harmonics in U with the time (U is the evolution operator (1)), or, in other words, the number of populated levels of the unperturbed system (one jolt covers $\approx 2k$ levels of the unperturbed system). Because of this, the number of θ harmonics in $\hat{p}_t = U^{+}(-i\hbar\partial/\partial\theta)U$ also increases as a power, which leads to $h = 0$ and nonexponential damping of the correlations. Since this property of U holds for almost all perturbations, it is natural to expect that other quantum systems which are stochastic in the classical limit will have vanishing Kolmogorov–Sinai entropy and power decrease of the correlations. This result indicates that the direct generalization of the concept of the Kolmogorov entropy to quantum systems [16, 17] is not so important as in classical systems.

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KINETICS OF RELAXATION TRANSITIONS BETWEEN MULTILEVEL QUANTUM STATES

A. A. Demidenko and É. G. Petrov

The nonequilibrium density matrix method is used in the approximation of strong "longitudinal" relaxation in each individual multilevel quantum state to study transitions induced by resonance interactions between levels belonging to different states of a quantum subsystem. The transition rates are found in the cases of weak and strong interaction of each of the levels of the subsystem with the thermal bath.

1. In the theoretical study of the transport of energy and charge in different physical, chemical, and biological systems (see, for example, [1-4]), it is frequently necessary to find the characteristic times $\tau_{\sigma\sigma'}$ of transitions between sets of levels σ and σ' in which internal transitions take place during short times τ_σ, $\tau_{\sigma'} \ll \tau_{\sigma\sigma'}$. For example, in the investigation of interterm transitions in a molecule, the vibrational levels of each term are the sets of levels, and the times τ_σ are the internal conversion times, which can be calculated explicitly in the harmonic approximation [2, 5]. In the investigation of electron transfer between molecules, one will take as the set of levels the vibrational levels of the molecules when the electron is at either a donor or an acceptor [3, 4].

The simplest way of finding $\tau_{\sigma\sigma'}$ – and the one usually employed – is to calculate the transition probabilities using Fermi's "golden rule" under the assumption of a Boltzmann distribution of the populations

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