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Transient Chaos in Quantum and Classical Mechanics

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Bogolubov's classical example of statistical relaxation in a many-dimensional linear oscillator is discussed. The relation of the discovered relaxation mechanism to quantum dynamics as well as to some new problems in classical mechanics is considered.

1. INTRODUCTION

In 1945 Bogolubov published a paper entitled "An Elementary Example of Relaxation to Statistical Equilibrium in a System Coupled to the Thermal Reservoir."[1] The model in question is specified by the Hamiltonian

$$\begin{aligned} H &= H_S + H_\Sigma + H_{S\Sigma} \\ &= \tfrac{1}{2}(p^2 + \omega^2 q^2) + \tfrac{1}{2} \sum_{n=1}^{N} (p_n^2 + \omega_n^2 q_n^2) + \varepsilon \sum_{n=1}^{N} \alpha_n q_n q \end{aligned} \tag{1}$$

It consists of a "probe" harmonic oscillator (H_S) weakly ($\varepsilon \to 0$) coupled ($H_{S\Sigma}$) to a "thermal reservoir" (H_Σ) made up of N also harmonic ("thermal") oscillators with some distribution in their frequencies ω_n and energies $E_n = \frac{1}{2}(p_n^2 + \omega_n^2 q_n^2)$.

Under the two assumptions (i) that the statistical properties of the thermal reservoir are described by the Gibbs canonical phase density

$$\rho_\Sigma = \exp\left(\frac{\psi - H_\Sigma}{T}\right) \tag{2}$$

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and (ii) that the distributions of α_n and ω_n admit the limit

$$\sum_n \frac{\alpha_n^2}{\omega_n^2} \to \int d\omega \, J(\omega), \qquad N \to \infty \tag{3}$$

where $J(\omega)$ is some continuous spectral density of the perturbation, Bogolubov proved that the probe oscillator also approaches the Gibbs distribution as $t \to \infty$. In other words, in the limit $N \to \infty$, an infinitely small subsystem H_S of dynamical system (1) exhibits statistical relaxation. If initially, at $t = 0$, the energy of this subsystem $E_S(0) = 0$, the relaxation takes the especially simple form[1]:

$$\rho_S = \frac{\omega}{2\pi T_S(t)} e^{-E_S/T_S(t)}, \qquad T_S(t) = T(1 - e^{-\gamma t}) \tag{4}$$

where the relaxation rate

$$\gamma = \frac{\pi}{2} \varepsilon^2 J(\omega) \tag{5}$$

In this Bogolubov's example, a certain *particular mechanism* of statistical laws, or of chaos (in modern language), was clearly and rigorously demonstrated for the first time. Previously, such a mechanism had been only implicitly and intuitively understood because of the very intricate and irregular motion of the dynamical system with an enormously large N. Following Ref. 2, we shall call this mechanism the *temporary, or transient, chaos.* The meaning of this term will become clear in Sec. 3. This approach developed since then and has now been made almost perfect by Bogolubov and his school, by the Prigogine school, and by many other scientists. Today it forms the foundations of statistical physics of macroscopic bodies. Various mathematical aspects of this problem have also been studied in detail today (see, e.g., Ref. 3), beginning from a classical work due to Khinchin.[4]

The keystone of the transient chaos mechanism, as Bogolubov is used to emphasize,[5] is the transition $N \to \infty$, which is called the thermodynamic limit in statistical physics. Some additional statistical hypotheses are also required for this mechanism to be efficient. In Bogolubov's example, they are specified by Eqs. (2) and (3). The first one, in particular, implies randomness and independence of the initial phases of thermal oscillators. It is thus clear that relaxation to the Gibbs distribution here is a particular case of the central limit theorem in probability theory (cf. Ref. 4).

It is worth mentioning that condition (2) is actually insignificant (see Sec. 4), including the random phase assumption. According to Kac's theorem,[6] the latter may be replaced by the requirement that the frequencies ω_n be incommensurable, or linearly independent. However, the absence of any initial correlations between the probe oscillator and thermal reservoir is essential. It is realized, in particular, if at the beginning the oscillator is in some determined dynamical state, say, $E_S(0) = 0$.

Recently, Bogolubov came back to his classical example in its quantum version.[5]

Presently, a remarkable peculiarity of Bogolubov's example is that the system (1) is completely (and trivially) integrable at any finite N. Such a system has a complete set of N commuting integrals of motion, and its trajectories fill up N-dimensional tori. Hence the motion is not even ergodic. Nevertheless, in the limit $N \to \infty$, the statistical relaxation does occur, which requires at least the mixing. Moreover, the relaxation is exponential in time, obeying (4), which is one of the strongest statistical properties according to modern ergodic theory. At present the possibility of such statistical properties in an infinite system which is completely integrable at any finite N has been rigorously proved indeed.[3] In Bogolubov's example it is explained by the fact that after the *earlier* transition to the limit $N \to \infty$ the perturbation spectrum of the probe oscillator becomes *continuous* [Eq. (3)], which is a necessary condition for the mixing. The importance of this transition was especially stressed even in the first paper of this series written by Bogolubov and his teacher Krylov in 1939 (see Ref. 7), where the Fokker–Planck–Kolmogorov diffusion equation has been derived in this way in both the classical and quantum cases.

Therefore, one may say that the relaxation in Bogolubov's example is a *relaxation in the continuous spectrum*, while the thermal reservoir H_Σ presents a dynamical model of external random noise. An important new question is what the statistical properties of Bogolubov's model (1) are at arbitrarily large but finite N. A related question is: Is the *relaxation in the discrete spectrum* possible, i.e., by taking the limits $N \to \infty$ and $t \to \infty$ ($\varepsilon \to 0$), not successively but simultaneously? We shall discuss these questions in Sec. 4.

2. DYNAMICAL CHAOS

In 1939, the same year when the article by Bogolubov and Krylov[7] was published, the papers by Hedlund and by Hopf appeared, which marked the beginning of modern ergodic theory (see, e.g., Ref. 9) based upon the property of the strongest (exponential) local instability of motion. By the end of the forties this new theory had already been applied by Krylov to the foundations of statistical physics.[10]

As there is no instability in Bogolubov's example, the new ergodic theory put forward a *different mechanism* for statistical laws in dynamical systems which is usually now called among physicists the *dynamical chaos* (stochasticity). Its most striking distinction from the transient chaos at $N \to \infty$ is just the fact that N may be not only finite but also very small.

In a Hamiltonian system, for example, it suffices to take $N > 1$ for chaos, including $N = 1.5$ (an oscillator with one degree of freedom driven by an external periodic perturbation). Generally, the chaos may occur even in a one-dimensional mapping such as the following, for instance (see, e.g., Ref. 11, Sec. 5.2c,d):

$$\varphi_{n+1} = k\varphi_n \bmod 1, \qquad z_{n+1} = z_n^k, \qquad z = e^{2\pi i\varphi} \tag{6}$$

where $k > 1$ is any integer. Curiously, the solution of this difference equation can be written explicitly:

$$z_n = z_0^{(k^n)}, \qquad \varphi_n = \varphi_0 k^n \bmod 1 \tag{7}$$

However, this does not help us at all to get rid of the chaos, which appears just upon the transition from a regularly growing but unphysical angle (phase) φ to the physical *direction* of vector z, i.e., to φ *mod 1*.

The mathematical theory of dynamical chaos has been developed in the works by Kolmogorov and his school, by Anosov and his pupils, and by many other researchers (see Ref. 9).

The significance of dynamical chaos is, first of all, that it extends statistical laws into a completely new domain of simple (small N) dynamical systems. Even though one cannot introduce "macroscopic" variables in such systems, and neither is there any "thermodynamic limit" here, their evolution is also described by some kinetic (particularly, diffusion) equation. In the case of a closed system it results in the relaxation to a microcanonical distribution for the whole system and to a Gibbs canonical distribution for any of its small subsystems (if N is large enough).

The ultimate origin of dynamical chaos is related to *continuity* of the phase space in classical mechanics. The exactly fixed (imaginarily!) initial conditions contain an infinite amount of information which gradually determines the whole motion via the mechanism of local instability.[12]

Is there any relation between the two sorts of chaos described above, which seem so different at first glance? The key to the solution of this problem lies in the following important property of dynamical chaos: Its motion spectrum is always *continuous* (at finite N!), i.e., just that for which the limit $N \to \infty$ is required in the theory of transient chaos. Now we are almost ready to answer the above question, but first let us see what happens with dynamical chaos in quantum mechanics.

3. QUANTUM PSEUDOCHAOS

The problem whether dynamical chaos is possible in quantum mechanics was first considered in the late forties by Krylov[10] and has been resolved by him in the negative. Since then his answer has not changed. The point is that the energy (frequency) spectrum of any quantum system *bounded in the phase space* is purely discrete, which implies an almost periodic temporal evolution of the system wave function $\psi(t)$. This is just opposite to the classical dynamical chaos.

Thus, we see that there is a far-reaching similarity between the quantum dynamics and that of a classical completely integrable system like Bogolubov's model (1). It is also clear that in both cases the number of independent frequencies N_ω, which determine the dynamics, rather than N, is essential. As $N \to \infty$, the number $N_\omega \to \infty$ as well, in both classical and quantum mechanics, which results in the transient chaos whose mechanism is actually the same in both cases, as has been established in the first paper by Bogolubov and Krylov.[7] However, in quantum mechanics there is another possibility, namely, at finite $N > 1$ (including small N), $N_\omega \to \infty$, which corresponds to the quasiclassical limit.

At any finite N_ω, true dynamical chaos is impossible. However, the fundamental correspondence principle requires, nevertheless, some transition from quantum to classical mechanics in general, and to the classical dynamical chaos, in particular. How does one resolve this apparent contradiction? The idea is[2] to introduce some characteristic time scales of the quantum evolution. The most important one seems to be the so-called diffusion (relaxation) time scale, which is given, according to Ref. 2, by the estimate: $t_d \sim \hbar\eta$, where η is the mean density of the system energy (or quasienergy) levels. The physical meaning of this scale is very simple and also relates to a fundamental uncertainty principle. Indeed, while $t \ll t_d$, the energy uncertainty $\Delta E \gg \eta^{-1}$ well exceeds the average level spacing, and the system does not yet "feel" the spectrum discreteness. Hence, the evolution is temporary, determined by a would-be continuous spectrum, and it *may* be the same as in the classical limit. Various numerical experiments[2,13,14] prove that it is just the case *indeed*, in spite of the absence of any strong local instability of motion, on scale t_d, in quantum dynamics.[13]

Numerical simulations also show that at $t \gg t_d$, the quantum diffusion completely vanishes[2,13–15] and turns into a stationary oscillation of $\psi(t)$ and into localization of the quantum state in momentum space, particularly on an energy surface.

In the case of a time-dependent perturbation, the localization always terminates the classical relaxation process. However, in a closed system with bounded energy surfaces the relaxation picture may be quite different.

Namely, if the localization length exceeds the size of the energy surface, any initial state has enough time for relaxation to a microcanonical distribution. This implies ergodicity of almost all eigenfunctions.[16] The condition for ergodicity is roughly given by the *discreteness parameter* of quantum spectrum

$$\kappa = \frac{t_d}{t_R} \sim \eta \cdot \hbar\gamma \gtrsim 1 \tag{8}$$

where $t_R = \gamma^{-1}$ is the classical relaxation time.

The temporal evolution of a quantum system is always almost periodic, even if its eigenfunctions are ergodic. Thus, the quantum chaos may be, at the most, a temporary imitation of the true randomness which is reached in the classical limit only. Hence the term *temporary*, or *transient*, *pseudochaos*.[2]

4. RELAXATION IN DISCRETE SPECTRUM

Now we come back to the classical example of Bogolubov, and attempt to answer the questions posed at the end of Sec. 1.

Consider first some fixed $N \gg 1$. Then, the perturbation spectrum for the probe oscillator in model (1) is discrete with some finite mean frequency density $\tau = N/\Delta$, where $\Delta \neq 0$ is a width of the full spectrum of thermal oscillators. The studies of quantum dynamics described above suggest the existence of a similar time scale $t_d \sim \tau$ on which the perturbation acts as if it were of a continuous spectrum with the density

$$J(\omega) = \frac{\alpha^2(\omega) \cdot \tau(\omega)}{\omega^2} \tag{9}$$

Hence, the probe oscillator would relax on this scale as in the limit $N \to \infty$, Eq. (4), provided $\gamma \ll \Delta$, the condition that is always satisfied as $\varepsilon \to 0$. However, the result of relaxation crucially depends on the classical discreteness parameter

$$\kappa = \gamma\tau \sim \left(\frac{\varepsilon\alpha\tau}{\omega}\right)^2 \lesssim N \tag{10}$$

which is quite similar to its quantum counterpart (8). The last inequality relates to the above condition $\gamma \lesssim \Delta$.

If $\kappa \gg 1$, the relaxation would be accomplished in spite of the spectrum discreteness, just as in quantum dynamics. Similarly, some residual oscillations of any relaxing quantity do generally persist because of its almost periodic dependence on time. Yet, the oscillation amplitude can be shown to decrease as $\kappa^{-1/2}$. Moreover, the oscillations may be efficiently suppressed by an appropriate time averaging. Here is also the answer to the second question in Sec. 1. We can take both limits, $N \to \infty$ and $t \to \infty$ ($\varepsilon \to 0$), simultaneously, provided that $\kappa \to \infty$ also, i.e., that $\varepsilon^2 N \to \infty$ if we keep $J = \text{const}$ ($\alpha^2 N = \text{const}$) or $\varepsilon N \to \infty$ for $\alpha = \text{const}$. If, instead, we kept $\kappa = \text{const}$ as $N \to \infty$, the relaxation would never be complete in the sense of a residual oscillation.

In the more interesting case $\kappa \ll 1$ the time scale τ is insufficient to heat the probe oscillator up to the temperature T. As $t \to \infty$ the average oscillator energy can be shown to increase only up to $\langle E_S \rangle \sim T\sqrt{\kappa} \ll T$.

The straightforward analogy to the quantum problem in Sec. 3 would lead to the estimate $\langle E_S \rangle \sim \kappa T$, which proves to be wrong. The point is that, for $\kappa \ll 1$, the energy $\langle E_S \rangle$ is essentially determined by just a single thermal oscillator with the minimal difference $|\omega_n - \omega|$, while for $\kappa \gg 1$ many ($\sim \tau\gamma \sim \kappa$) oscillators do contribute to $\langle E_S \rangle$.

To make the similarity with quantum mechanics still closer, let us somewhat complicate Bogolubov's example by introducing a linear coupling among all the oscillators ($\alpha_n \to \alpha_{mn}$), and consider their simultaneous relaxation. Mathematically, this problem is reduced to the diagonalization of the matrix

$$H_{mn} = \omega_n^2 \delta_{mn} + \varepsilon a_{mn} \tag{11}$$

by a rotation of coordinate axes: $q_n \to Q_m$, where $q_n = b_{nm} Q_m$ with some orthogonal matrix b_{nm} and the normal coordinates Q_m. But this is just one of the basic problems in random matrix theory, a statistical theory of complex quantum systems which explicitly takes account of the discreteness of quantum spectrum (see, e.g., Ref. 17).

Coming back to our mechanical problem, we first observe that condition (2) is insignificant for Bogolubov's example. In Ref. 1 it was applied to obtain the relation $\langle E_n \rangle = T$ only (cf. Ref. 7). Therefore, the relaxation (4) would occur for any (nonsingular) ρ_Σ, the only difference being that the final temperature of the probe oscillator would be determined now by the average energy of thermal oscillators at frequency $\omega_n \approx \omega$, that is, $T \to \langle E_n \rangle_{\omega_n = \omega}$. Thus, the relaxation becomes local in frequency.

A similar local relaxation also occurs for the model (11), provided $1 \lesssim \kappa \lesssim N$, (10). In the corresponding quantum problem, the condition $\kappa \gtrsim 1$ implies that the perturbation $\varepsilon\alpha$ exceeds the mean spacing of unperturbed eigenvalues $\delta\omega^2 \sim \omega\, \delta\omega \sim \omega\Delta/N$. This results in a breakdown of perturbation theory, in intense transitions among neighboring unperturbed states, and in their strong mixing by perturbation. It is a necessary condition for the quantum pseudochaos known as Shuryak's criterion.[18] In the present case, yet not always, it coincides with the other condition (8) related to the diffusion time scale.

The local relaxation produces the canonical distribution of oscillators with a frequency-dependent temperature $T(\omega)$. What are the conditions for the global relaxation to a unique temperature over the whole frequency band Δ? A sufficient condition would be $\gamma \gtrsim \Delta$, or

$$\varepsilon^2 N \frac{\alpha^2}{\omega^2 \Delta^2} \sim \frac{\kappa}{N} \gtrsim 1 \tag{12}$$

which implies an efficient interaction among *all* the oscillators and, hence, their simultaneous relaxation. This global relaxation is, of course, quite different from the local one, (4), as a necessary condition for the latter ($\gamma \not\ll \Delta$) is just violated according to Eq. (12).

The global relaxation in a linear oscillator was apparently first observed by Ford *et al.*[19] in numerical experiments with a version of model (11) and for $\Delta = 0$, that is, for a degenerate (resonant) unperturbed system with all the frequencies equal. In this case, condition (12) is obviously satisfied, but there is no room for the local relaxation.

In the quantum problem the condition (12) means that perturbation mixes up all the unperturbed states and not just a few neighboring ones as for $\kappa \gtrsim 1$ only. This may be elucidated in two ways.

First, one may apply Shuryak's criterion for transitions among arbitrary unperturbed states. Since their mean separation is $\delta\omega^2 \sim \omega\Delta$, while the effective perturbation $V \sim \varepsilon\alpha\sqrt{N}$ (we assume matrix elements α_{mn} to be random and independent), the ratio $V/\delta\omega^2 \sim (\gamma/\Delta)^{1/2} \gtrsim 1$, which is just the condition (12).

Strong mixing of all the unperturbed states implies ergodicity of the exact eigenfunctions in the unperturbed basis. The ergodicity condition for matrices of the type (11) with a small random perturbation is obtained in the random matrix theory and does coincide with Eq. (12), indeed (see, e.g., Ref. 17, Chap. IV G, where $\alpha \sim \omega^2 \sim \Delta^2$). Such a condition had first been obtained in numerical experiments[20] and then explained by Dyson[21] via a very nice and physical picture of the eigenvalue "dynamics" in ε, i.e., as the perturbation grows. It gives another interpretation of condition (12). Indeed, for random and independent α_{mn}'s, the resulting displacement of unperturbed eigenvalues is $\delta\omega_n^2 \sim \varepsilon\alpha\sqrt{N}$. Then, the condition (12) implies $\delta\omega_n \gtrsim \Delta$, which means that each eigenvalue has "crossed" all the others in the process of "motion" and, hence, has been mixed up with any other unperturbed state.

The same interpretation holds for the classical problem as well. Here successive "crossings" of the frequencies of normal oscillators also have the result that the latter become a superposition of more and more unperturbed oscillators.

5. CONCLUSION

A simple Bogolubov's example, which exposes the mechanism of transient chaos in classical statistical mechanics, turns out to be even more instructive in the problem of quantum chaos where that mechanism is the only one possible. In particular, the quantum random matrix theory reveals a far-reaching analogy to a much less developed (however, strange it may seem!) theory of the classical many-dimensional linear oscillator.

Well, and what about a nonlinear classical oscillator? Quantum mechanics may help here, too, if the oscillator is a completely integrable one like, for example, the Toda lattice (see, e.g., Ref. 11, Sec. 1.3c). The crucial point here is the mixing up of many linear (unperturbed) modes, which requires a sufficiently high excitation energy. Indeed, numerical experiments by Ford and co-workers[22] revealed the energy sharing among the linear modes under this condition.

There are also other applications which are much closer to quantum dynamics. These are linear waves in nonhomogeneous dispersive media, in a plasma, for example,[23] or in waveguides and resonators.[24] It is instructive to mention that in the latter case an apparently academic Sinai's problem on the classical billiard dynamics[25] turns out to be of practical importance. In all those systems, chaos is possible[23,24] in the geometrical-optics approximation, which is the analog to the quasiclassical approximation in quantum mechanics. Note, however, that this chaos is only a transient one, i.e., a pseudochaos.

The last but not least application of the transient chaos concerns the global problem of numerical experiments in classical dynamical chaos. A principal limitation here is the discreteness of any quantity in the digital computer. This calls forth a naive analogy with the discrete phase space in quantum mechanics. As a matter of fact, the computer dynamics proves to be even more "quantal," since any dynamical trajectory on a discrete lattice eventually becomes just periodic as compared to an almost periodic quantum $\psi(t)$. This problem was discussed recently in Ref. 2, for example, but actually it has already been known for a long time in the theory and practice of the computer pseudorandom number generators. Such generators (algorithms) appeared in the early fifties, well before the theory of dynamical chaos was developed. At that time the term "pseudo" was related to the widespread belief in the impossibility, in principle, of any "true" randomness in dynamical systems. Today we know that this is wrong (Sec. 2). However, the term "pseudo" remains and now relates to the fact that in a digital computer (as well as in quantum mechanics!) only a temporary imitation of true dynamical randomness is possible. For example, map (6) in real numbers does produce a *random* sequence φ_n (mod 1). Yet, the same map in *integers* (the most widespread and the best generator) provides a *pseudorandom* string of integer φ_n's which is actually periodic. Moreover, as is shown in Ref. 2, a simple discretization of the action variable in a classical chaotic dynamical system ($J \to n \cdot \Delta J$) qualitatively mimics the quantum pseudochaos with $\hbar = \Delta J$!

Thus, the phenomenon of transient pseudochaos, which was once taken as the basis of classical statistical physics, now has been reborn in quantum mechanics and may help again in the solution of new problems in classical dynamics.

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