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SELF-STOCHASTICITY IN BOUNDARY VALUE PROBLEMS OF QUANTUM MECHANICS

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On the example of an initial-value boundary problem for the Schrödinger equation, a methodological problem of quantum mechanics has been discussed. It is shown that quantum mechanical problems can be reduced to difference equations with continuous time for which there exist so-called self-stochastic solutions. Hence, such solutions exist for quantum problems. These solutions are random function as time is large. It is shown that the Sharkovsky metric can be applied for computer simulation of limit distributions of random wave functions.

Keywords: quantum mechanics, initial boundary value problem, difference equations

There is always another way to say the same thing that doesn't look at all like the way it was said before.

Richard Feynman

1. Introduction

Nowadays physical world view contains a substantial blank space. Namely, there is no bridge between the sub-microscopic level of quantum mechanics and the macro-world of classical physics. It is known that there is the smallest change value in nature (see [1]). From this statement, it follows that motion is «fuzzy». Next, classical constants (for example, the speed of light c or the gravitational constant G) do not allow definition of the scales of length or time. Thus, classical physics does not provide measurement scales, that is: «Classical physics alone cannot be used to build any measurement device» [1, p. 16]. Moreover, every failure of classical physics can be explained by the discovery made by Max Planck, 1899: «In nature, action value smaller then $\hbar = 1.06 \cdot 10^{-34}$ J·s are not observed». This is so-called fundamental quantum principle, which passes experimental tests. The constant \hbar is called the quantum of action or the Planck constant. The quantum principle states that there is no experiment, which can measure an action. Hence, in nature, a change smaller then \hbar cannot be observed. Thus, all consequence of this «strange» smallest change may be applied to nature.

Let us consider the Schrödinger equation

$$-i\hbar \frac{\partial \psi}{\partial t} = \frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \quad (1)$$

where $\psi := \psi(x, t) : R^2 \rightarrow C$, C is a complex space, ψ is an unknown function, \hbar is the Planck constant. Let us divide the two parts of the equation by mv^2 where m is the mass of particles, v is their velocity and $p = mv$ is an impulse. Further, we introduce $\bar{t} = t/\tau$, τ is the relaxation time of a wave function to some equilibrium, and we consider a dimensionless constant $h = \lambda/\nu\tau$. As a result, we obtain the dimensionless equation:

$$-ih \frac{\partial \psi}{\partial \bar{t}} = \frac{1}{2} h^2 \frac{\partial^2 \psi}{\partial x^2}. \quad (2)$$

For example, we can consider the functional two-point boundary conditions

$$\psi(0, t) = \theta \psi(l, t) \quad (3)$$

with θ being a real or complex parameter. But our aim is considering of nonlinear boundary conditions instead of the linear boundary conditions

$$\psi(0, t, h) = \Phi[\psi(l, t, h)] \quad (4)$$

where $\Phi : C \rightarrow C$ is a nonlinear structural stable map, with the initial condition added:

$$\psi(x, 0, h) = \psi_0(x, h), \quad 0 < x < l \quad (5)$$

where $h > 0$ is a small parameter.

We assume that conditions

$$\psi(0, 0, h) = \Phi[\theta, \psi(l, 0, h)], \quad \psi(0, l, h) = \Phi[\theta, \psi(l, l, h)] \quad (6)$$

and similar conditions for second derivatives at points $(0;0)$ and $(l;0)$ are satisfied. This ensures the existence of solutions of $C^2[(0,l) \times [0,t_0)]$ -class. Of course, real and imaginary parts of the map Φ are of C^2 -class. This fact ensures that the map $\Phi : C \rightarrow C$ is structurally stable. It means that the related map $G : R^2 \rightarrow R^2$ is structurally stable, too. Thus, the spectrum $\sigma(TG^r) \cap \{z : |z|=1\} = \emptyset$ where \emptyset is an empty set.

Further we assume that $h > 0$ is a small parameter, and we consider the problem with accuracy of $O(h^2)$, where $O(h^2) \rightarrow 0$ as $t \rightarrow +\infty$. We find solutions in the form

$$\psi(x, t, h) = \exp\left(\frac{iS(x, t)}{h}\right) \varphi(x, t, h), \quad (7)$$

where $S(x; t)$ is the real phase, and $\varphi(x; t; h)$ is the real amplitude. (Below, the parameter h will be omitted where it will not cause imperfect understanding.)

We assume that $C^0([0, l] \times [0, +\infty))$ is the space of bounded continuous functions, and C^2 is the space of twice differentiable functions with the norm: $\|f\|_{C^2} = \sum_{k=0}^2 \sup \|f^k\|$, where $\|f_0\|$ is the norm in $C^0([0, l] \times [0, +\infty))$. The function $\psi \in C^2$ if its real and imaginary parts belong to $C^0([0, l] \times [0, +\infty))$. Then there is the following convergence in C^2 -norm:

$$\|S(x, t)\|_{C^2} \Rightarrow \left\| \Phi_1 \left[p_1 \left(t - \frac{x}{p} \right) \right] \right\|_{C^2} \quad (8)$$

where $p_1(\zeta)$ is $2^N l/p$, that is a periodic piecewise constant distribution with a finite number of points of discontinuities Γ . Here, $\Gamma = \rho^{-1}(D)$, $D = \bigcup_{n>0} G^{-n}(A^\pm)$, and A^\pm is a set of saddle points of co-dimension one, and $\rho(\zeta) = (S_0(\zeta), \varphi_0(\zeta))$ is an initial curve in R^2 , which is determined by the initial data of the boundary problem, and N is the least common multiple of the map $G: (S, \varphi) \rightarrow (\Phi_1(S, \varphi), \Phi_2(S, \varphi))$.

2. Method of reduction of the problem to a system of integro-difference equations

Now we return to the problem, which can describe the behavior of white and black solitons in an optical resonator with surface feedback [2–6]. Indeed, substituting (7) in equation (2), we obtain that

$$\left(\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S)^2 \right) \varphi + (-ih) \left(\frac{\partial S}{\partial x} \frac{\partial \varphi}{\partial x} + \frac{\partial \varphi}{\partial t} + \frac{1}{2} \varphi \Delta S \right) + \frac{(-ih)^2}{2} \Delta \varphi = 0. \quad (9)$$

We find solutions with accuracy of $O(h^2)$ so that

$$\left(\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S)^2 \right) \varphi + (-ih) \left(\frac{\partial S}{\partial x} \frac{\partial \varphi}{\partial x} + \frac{\partial \varphi}{\partial t} + \frac{1}{2} \varphi \Delta S \right) = 0. \quad (10)$$

Then we obtain the Hamilton–Jacobi equation [7–9]:

$$\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S)^2 = 0. \quad (11)$$

The boundary conditions can be written in the form:

$$\cos S\varphi_{x=0} = \Re\Phi(S; \varphi)_{x=l}; \quad \sin S\varphi_{x=0} = \Im\Phi(S; \varphi)_{x=l} \quad (12)$$

where \Re and \Im are real and imaginary parts of a complex number.

Let us denote $F_1 := \Re\Phi$ and $F_2 := \Im\Phi$. Then it follows from (12) that

$$\varphi_{x=0}^2 = F_1^2(S, \varphi)_{x=l} + F_2^2(S, \varphi)_{x=l}, \quad (13)$$

$$\tan S_{x=0} = F_1^2(S, \varphi)_{x=l} / F_2^2(S, \varphi)_{x=l}. \quad (14)$$

We define functions $\Phi_1 := +\sqrt{F_1^2 + F_2^2}$ and $\Phi_2 := \arctan F_2^2 / F_1^2$. Then the boundary conditions (4) can be written as

$$\varphi_{x=0} = \Phi_2(S, \varphi)_{x=l}, \quad (15)$$

$$S_{x=0} = \Phi_1(S, \varphi)_{x=l}. \quad (16)$$

For simplicity, initially we consider the case of $\Phi_2 := \Phi_2(\varphi)$ and $\Phi_1 := \Phi_1(S)$.

The general case can be treated in a similar way.

Thus, for the Hamilton–Jacobi equation we have the boundary conditions

$$S(0, t) = \Phi_1[S(l, t)] \quad (17)$$

and for the transport equation

$$\frac{\partial \varphi}{\partial t} + p \frac{\partial \varphi}{\partial x} + \frac{\partial^2 S}{\partial x^2} \varphi = 0 \quad (18)$$

we have the boundary conditions

$$\varphi(0, t) = \Phi_2[\varphi(l, t)]. \quad (19)$$

Here maps $\Phi_1, \Phi_2 \in C^1(I \rightarrow I)$ are structurally stable, and I is an open closed interval. The structural stable maps form an open dense subset (see [10], p. 233).

In order to solve equations, we use the method of characteristics. To do this, we consider the Hamilton system of ordinary difference equations with Hamiltonian $H(x, p) = p^2/2$ as

$$\dot{x} = \frac{\partial H}{\partial p} = p, \quad \dot{p} = -\frac{\partial H}{\partial x} \quad (20)$$

with the initial conditions

$$x(0) = x_0, \quad p(0) = \frac{\partial S}{\partial x}(x_0) = p. \quad (21)$$

For a given constant p , the function $x := x(p; t)$ is the solution of equation

$$p - \frac{\partial S(x, t)}{\partial x} = 0 \quad (22)$$

where p can be considered as an additional coordinate in $(x; p; t)$ -space. Then on the characteristics $dx(p; t) = p$, we have the equation

$$\begin{aligned} \frac{dS(x(t, p), t)}{dt} &= \frac{\partial S(x(t, p), t)}{\partial t} + \frac{\partial S(x(t, p), t)}{\partial x} \frac{dx(t, p)}{dt} = \\ &= -H(p) + p \frac{dx(t, p)}{dt}. \end{aligned} \quad (23)$$

By integration along characteristics $dx/dt = p$ and with the help of boundary conditions, the problem can be reduced to the difference equations:

$$S(x, t) = \Phi_1 \left[S(x, t - l/p) + \frac{p}{2}(l - x) \right] + \frac{p}{2}l. \quad (24)$$

We can solve this difference equation as $x = 0$. Then

$$S(l, t) = \Phi_1 \left[S(l, t - l/p) \right] + \frac{p}{2}l. \quad (25)$$

If Φ_1 is a unimodal map, then solutions tend to piecewise constants $2^N l/v$ that are periodic functions with finite or infinite points of discontinuities on a period. N is the least common multiple of attractive circles of the map Φ_1 [10]. If $\Phi_1; = Id$, where Id is an identical map, the solutions are unstable.

Next, from relation

$$S(l, t) = S(0, t - l/p) + \frac{p}{2}l \quad (26)$$

it follows that the limit function $S(0; t)$ is also a piecewise constant periodic function, and from the relation

$$S(x, t) = S(0, t - x/p) + \frac{p}{2}x \quad (27)$$

we find the limit phase distribution in the bulk.

3. Asymptotic distributions of amplitudes

The second equation follows from the integration of the transport equation (19), which can be written as [9,11]:

$$\frac{d\varphi}{dt} = -\frac{1}{2} \frac{\partial^2 S}{\partial x^2} \varphi. \quad (28)$$

Integration of this equation from point (x, t) to point $(x, t - l/p)$ with the help of the boundary conditions for amplitude results in equation (27). On the other hand, this equation has a solution

$$\frac{d\varphi}{dt} = -\frac{1}{2} \frac{\partial^2 S}{\partial x^2} \varphi \text{ at } dx/dt. \quad (29)$$

After multiplying by φ , this equation can be written as

$$\varphi(x(t), t) = \varphi(x(t_0), t_0) \exp \left(-\int_{t_0}^t \frac{\partial^2 S}{\partial x^2} [p(s-t) + x, s] \varphi [p(s-t) + x, s] ds \right). \quad (30)$$

Now we can find the phase $S(x, t)$ in this equation. Indeed,

$$S(x, t) = S(0, t - x/p) + \frac{1}{2} px. \quad (31)$$

Further, using the boundary conditions for the phase, we obtain from (31) that

$$S(l, t) = S(l, t) + \frac{p}{2} l = \Phi_1 [S(l, t - l/p)] + \frac{p}{2} l. \quad (32)$$

This equation has an asymptotic solution $S(l, t) \Rightarrow p_1(l, t)$. Then we obtain from (32) that $S(l, t) \Rightarrow \Phi_1 [p_1(l, t - x/p)] + px/2$. Then

$$\begin{aligned} p^2 \frac{\partial^2 S}{\partial x^2} &= \Phi_1'' [S(l, t - x/p)] [S'(l, t - x/p)]^2 + \\ &+ \Phi_1' [S(l, t - x/p)] [S''(l, t - x/p)] \end{aligned} \quad (33)$$

where we used the relation

$$\begin{aligned} \frac{\partial^2 S}{\partial x^2} [p(s-t) + x, s] &= S''(0, t - x/p) = \Phi_1'' [S(l, t - x/p)] \times \\ &\times [S'(l, t - x/p)]^2 + \Phi_1' [S(l, t - x/p)] [S''(l, t - x/p)]. \end{aligned} \quad (34)$$

$S(l, t - x/p)$ tends to $2^{N_1}(t - x/p)$ periodic function $p_1(l, t - x/p) \in A_1^+$, where A_1^+ is a set of attractive points of the map Φ_1 . Here index μ is omitted in the map $\Phi_{1,\mu}$. Then we obtain the equation

$$\varphi(x(t), t) = \varphi(x(t_0), t_0) \exp \left[-S''(0, t - x/p) \int_{t_0}^t \varphi [p(s-t) + x, s] ds \right]. \quad (35)$$

We assume that $S(l, t) = A_1^+ + \varepsilon S(\tilde{l}, t)$ where $\varepsilon > 0$ is a small parameter. Then lumbarization of difference equation (32) at every point $a \in A_1^+$ results in equation

$$S(\tilde{l}, t) = \Phi_1'(a) S(l, \tilde{t} - l/p) \quad (36)$$

where $|\Phi_1'(a)| < 1$. Solutions of these equations are $S(l, t) = \exp(kt)$ where $k = \frac{p}{l} \ln |\Phi_1'(a)|$. Hence, in the vicinity of the point $a \in A_1^+$, equation (35) can be written as

$$\varphi(x(t), t) = \varphi(x(t_0), t_0) \exp \left[-k^2 \exp(t - x/p) \int_{t_0}^t \varphi[p(s-t) + x, s] ds \right]. \quad (37)$$

Since $k < 0$, we can use the approximation $e^z \approx 1 - z$ and rewrite (37) in the form:

$$\varphi(x(t), t) = \varphi(x(t_0), t_0) \left[1 + k^2 \exp(t - x/p) \int_{t_0}^t \varphi[p(s-t) + x, s] ds \right]. \quad (38)$$

Then, in the class of bounded functions $\varphi \in C^2$, the last term in (38) can be neglected, because

$$\left| k^2 \exp(k(t - x/p)) \int_{t_0}^t \varphi[p(s-t) + x, s] ds \right| \leq k^2 \exp(k(t - x/p))(t - t_0) M \quad (39)$$

where $M = \sup |\varphi(x, t)|$ at $(x, t) \in [0, l] \times R^+$, and $k^2 \exp(k(t - x/p))(t - t_0) \rightarrow 0$ as $t \rightarrow +\infty$. It means that the function $\varphi(x(t), t) = \varphi(x(t_0), t_0)$ asymptotically. Hence, we have

$$\varphi(l, t) = \varphi(0, t - l/p) = \Phi_2[\varphi(l, t - l/p)]. \quad (40)$$

This equation has asymptotically $2^{N_1} l/p$ -periodic piecewise constant distributions $p_2(t) \in A_2^+$ where A_2^+ is a set of attractive points of the map $\Phi_2 \in C^2(I, I)$.

4. Reduction of initial boundary value problems to difference equations with continuous time

It is known that many problems of mathematical physics may be reduced to the study of asymptotic behavior of ID map $f: I \rightarrow I$ where I is an open bounded interval. In this case, the main role is played by the separator D of the map

$$D(f) = \left\{ y \in I : \text{trajectories of } f^n(y), n = 0, 1 \text{ are unstable} \right\}. \quad (41)$$

The term separator can be explained by the fact that the points of $D(f)$ set separate the basins of attractive circles of map f . Then for any point $y^* \in D(f)$, there is a number $d > 0$ such that for any $\varepsilon > 0$ there is a point $\tilde{y} \in (y^* - \varepsilon, y^* + \varepsilon) \cap I$ and a number m such that

$$\left| f^m(y) - f^m(\tilde{y}) \right| > d. \quad (42)$$

Next, if there is a set $D_{\text{sen}}(f)$ such that

$$L = \inf_{y \in D_{\text{sen}}(f)} d(y) > 0 \quad (43)$$

then

$$\sup \left| f^m(y) - f^m(\tilde{y}) \right| > L, \quad \tilde{y} : 0 < |y - \tilde{y}| < \varepsilon, \quad n > N \quad (44)$$

for any $\varepsilon > 0$ and $N > 0$. In this case, map f is sensitive to the initial data or sensitive map, and L is a constant of sensitivity.

It means that in dynamic systems, action values larger of L are not 'observed'. Thus we have the smallest action value L . We call this situation sensitive principle in classical mechanics.

Now we return to the discussion of the quantum principle. Similarly, it follows from the quantum principle that smaller change values can never be observed (see [1]). But it follows from classical mechanics that a small error of computer simulation leads to the fact that, for large times, there is the horizon of unpredictability. The corresponding trajectories are deterministic, but some of them are unpredictable. The sensitive trajectories cannot be ignored because a set of the initial data, which produce such trajectories, contains an open set (in C^0 -metric). The separator

$$D_n(f, \varphi) = \left\{ t \in (n, n+1) : \varphi(t-n) \in D_{\text{sen}}(f) \right\} \quad (45)$$

has an additional measure $D_{\text{sen}}(f)$ if an initial function $\varphi(t)$ is nonsingular with the property that measure $\text{meg}^{-1}(B) = 0$ for any set B of the Lebeque measure zero.

Next, all jumps of points of trajectories on interval Δt must be observed, as \hbar is small. But some of them can be observed only macroscopically, and only for a long period or for many particles average (see [1]). Thus, the difference between the action values S at an interval Δt can not vanish, so that

$$\left| S(t + \Delta) - S(t) \right| \geq \frac{\hbar}{2} \quad \text{and} \quad \Delta E \Delta t \geq \frac{\hbar}{2} \quad (46)$$

where E is the energy of a dynamic system. Next, there is the relation

$$\Delta x \Delta p \geq \frac{\hbar}{2} \quad (47)$$

where x is a position, and p is a momentum. The indeterminacy relation implies that measurement precision is limited. Since $p = \hbar/\lambda$, where λ is de Broglie wave, then relation (47) can be written as

$$\Delta x' \Delta l \geq \frac{\Delta \lambda}{2}. \quad (48)$$

5. Application example

Let us consider the map

$$f : z \rightarrow 4z(1-z), \quad z \in [0,1] \quad (49)$$

to which the origin quantum problem can be reduced with accuracy $O(\hbar^2)$. This map has the property: for any open interval $I \subset [0,1]$, there is N^* such that $f^n(I) = [0,1]$ for $n > N^*$. This means that for any $x \in [0,1]$ and $\varepsilon > 0$ there is t^* such that

$$S^t[\varphi](V_\varepsilon(x)) = [0,1] \quad \text{as } t > t^* \quad (50)$$

where S^t is a corresponding dynamical system, which is determined with accuracy $O(\hbar^2)$ for the given quantum problem, and $V_\varepsilon(x)$ is a neighborhood of point x . If $\varepsilon < \varepsilon^*$, where ε^* is a computer precision, then the computer recognizes $V_\varepsilon(x)$ as a «single point». As a result, the value $V_\varepsilon(x)$ is equal to anyone of the numbers on $[0;1]$ according to which implementation of f in the code is used (see [12]). In this case, we say that trajectories $S^t[\varphi]$ are out of predictability horizon for deterministic boundary value problems, and these trajectories are out of predictability horizon for quantum boundary value problems with accuracy $O(\hbar)$.

6. The Sharkovsky metric

Define a space $\mathfrak{R}(R^*; I)$ and let a function $\zeta \in \mathfrak{R}$. Define a family of metrics on \mathfrak{R}

$$\rho^\oplus(a, l)[\zeta_1, \zeta_2] = \sup_{\varepsilon > 0} \min \left(\varepsilon, \sum_{r=1}^{\infty} \frac{1}{a^r} \sup_{(z, i) \in I^r \times [0, l]^r} \left| F_{\zeta_1}^{r, \varepsilon}(z, \tau) - F_{\zeta_2}^{r, \varepsilon}(z, \tau) \right| \right) \quad (51)$$

where $a \geq 1$ and $l > 0$ are parameters, $F_{\zeta_2}^{r, \varepsilon}(z, \tau)$ are averaging of r -dimensional function of distributions of functions $\zeta(t)$ on ε -space of points $[0; l]^r$, so that

$$F_{\zeta}^{r,\varepsilon}(z, \tau) = \frac{1}{\text{meq } V_{\varepsilon}(\tau)} \int_{V_{\varepsilon}(t_1)} \dots \int_{V_{\varepsilon}(t_r)} F_{\zeta}(z_1, \dots, z_r, \theta_1, \dots, \theta_r) d\theta dz \quad (52)$$

where

$$V_{\varepsilon}(\tau) = V_{\varepsilon}(t_1) \times \dots \times V_{\varepsilon}(t_r), \quad V_{\varepsilon}(t_i) = (t_i - \varepsilon_i, t_i + \varepsilon_i) \quad (53)$$

and τ_1, \dots, τ_r are coordinates of point $[0; I]^r$, and z_1, \dots, z_r are coordinates of point $z \in I^r$. This metric is called Sharkovsky metric [13,14]. As shown above, for difference equations with continuous time (and, hence, for the quantum boundary problem), unpredictable solutions are typical as the time is large. These solutions can be described (with accuracy $O(\hbar)$) by the Sharkovsky metric. Then for the quantum problem there is a limit statistical process $P_{\varphi}(t)$ such that P_{φ} is a periodic random process with period p (see [12]). For example, $P_{\varphi}(t)$ is a stationary random process if $p = 1$, if the initial function φ is monotone.

Thus, for large time, deterministic solutions are similar to random process. In this case, ε -averaging distribution u_{φ} of the quantum problem are characterized by ε -averaging distributions P_{φ} . Moreover, if ε is not small, then ε -averaging distributions can be described by usual (not averaging) distributions. In this case, we enter in sphere of usual (classic) mechanics. Hence, we have «continuous» transition from quantum to classic mechanics. Besides, $\varepsilon > \varepsilon^*$ is required, where ε^* can be written as a composition of the minimal time Δt and the minimal size ΔL for quantum system. Moreover, the Sharkovsky metric allows to measure some quantities as precisely as possible in mathematical problems of quantum mechanics (see [1], p. 28). Next, it follows from this metric that measurement accuracy is limited, that is an «observer» cannot be microscopic that is the main condition of quantum mechanics, which follows from the constant \hbar (see [1]). As noted in [1]: «How can a system filter out the small and the large, and let the middle pass through?». The dynamic system implies some kind of measuring the frequency. But dynamic systems of classical physics do not allow measuring time or length. Now classical physics cannot explain any characteristic length or time scale observed in nature. The classical constants of nature do not allow defining length or time scales. In nature, there is always some action. It means that from mathematical point of view, the nature must be described by discrete dynamic systems. It can be called «the quantum principle» in mathematics.

Thus, self-stochasticity [3,7,8,10,12,15–18] in quantum dynamical systems means that there is a completion of phase space with random functions, which are determined with accuracy $O(\hbar^2)$, so that the system has a set of trajectories and, correspondingly, «attractor» of the problem contains wave functions.

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САМОСТОХАСТИЧНОСТЬ В КРАЕВЫХ ЗАДАЧАХ КВАНТОВОЙ МЕХАНИКИ

Обсуждается методологическая проблема квантовой механики на примере краевой задачи с начальными условиями для уравнения Шредингера. Показано, что квантовомеханические задачи могут быть сведены к разностным уравнениям с непрерывным временем, для которых существуют так называемые самостохастические решения. Следовательно, такие решения существуют и для квантовых задач. На больших временах эти решения являются случайными функциями. Показано, что метрика Шарковского может быть применена для компьютерного моделирования предельных распределений случайных волновых функций.

Ключевые слова: квантовая механика, начально-краевая задача, разностные уравнения