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Analysis of Traveling and Standing Waves in the DNA Model by Peyrard-Bishop-Dauxois

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Abstract
The model by Peyrard – Bishop – Dauxois (the PBD model), which describes the DNA molecule nonlinear dynamics, is considered This model represents two chains of rigid disks connected by nonlinear springs. An interaction between opposite disks of different chains is modeled by the Morse potential. Solutions of equations of motion are obtained analytically in two approximations of the small parameter method for two limit cases. The first one is the long-wavelength limit of traveling waves, when frequencies of vibrations are small. Dispersion relations are obtained also for the long-wavelength limit by the small parameter method The second case is a limit of high frequency standing waves in the form of out-of-phase vibration modes. Two such out-of-phase modes are obtained; it is selected one of them, which has the larger frequency. In both cases systems of nonlinear ODEs are obtained Nonlinear terms are presented by the Tailor series expansion, where terms up to third degree by displacement are saved The analytical solutions are compared with checking numerical simulation obtained by the Runge – Kutta method of the 4-th order. The comparison shows a good exactness of these approximate analytical solutions. Stability of the standing localized modes is analyzed by the numerical-analytical approach, which is connected with the Lyapunov definition of stability.

Keywords
PBD model, long-wavelength approximation, out-of-phase vibration modes

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Introduction

Research of wave propagation in the DNA molecule is one of important problems of the modern nano-technology. It is associated with design of perspective nano-robots constructed on the basis of the DNA molecules.

Detailed review on models of nonlinear dynamics of the DNA is done in the book [1] and in reviews [2,3]. One of the most successful models of the DNA molecule is the PB model, proposed by Peyrard and Bishop [4]. Two chains of DNA are presented by the model with two connected chains of rigid disks where interactions of opposite disks of different chains are described by the Morse potential. The staking interactions of the neighboring disks inside the each chain are linear. The problem of chains deviation was considered, so, the only one-dimensional dynamics is analyzed by the PB model. To have more adequate description of the staking introduction the model by Peyrard-Bishop- Dauxois (PBD model) was proposed where the anharmonic potential is introduced to describe this interaction [5]. Processes of the wave propagation are investigated later and presented in publications [1-3]. In particular, the discrete breathers are considered in PB and PBD models [6,7].

In this paper the investigation of some types of waves is made in the framework of the PBD model which is presented in Section 1. In Section 2 traveling waves in the long-wavelength limit are constructed by the small parameter method. Analytical solutions are compared with results of numerical simulation. Dispersion relations are obtained for the long-wavelength limit by the small parameter method too. Besides, in Section 3 the most high frequency standing waves are constructed in the form of anti-phase vibration modes. In Section 4 a stability of the localized standing waves is considered by the numerical-analytical approach which is a consequence of the well-known Lyapunov definition of stability. Boundaries of the stability/ instability regions in the space of parameters are obtained.

1. Model by Peyrard-Bishop-Dauxois

As it was written above, the PBD model is presented by two connected chains of rigid disks connected by longitudinal and transversal springs (Fig.1).

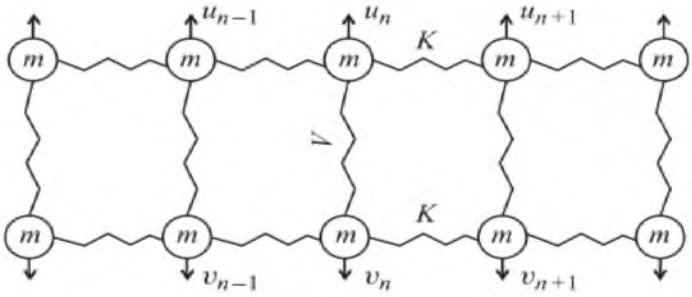


Figure 1. Model of DNA by Peyrard-Bishop- Dauxois (PBD model)

Interaction of nodes of different chains is modelled by the Morse potential, $V = d(\exp(-a(u_n - v_n)) - 1)^2$, which imitates hydrogen bonds between bases of complementary pairs. Here d is the energy of dissociation of polynucleotide chains; a is the parameter which is inverse to distance between disks (so-called space scale of the potential). Using the change of variables, $z_n = \frac{u_n + v_n}{\sqrt{2}}$, $y_n = \frac{u_n - v_n}{\sqrt{2}}$, one obtains the equations of motion of the PBD model [5] in the form:

$$\begin{aligned}
\frac{d^2 z_n}{dt^2} &= S(z_{n+1} - 2z_n + z_{n-1}) + S\rho\left\{e^{-\gamma(z_{n+1}+z_n)}(z_{n+1} - z_n)\left[\tfrac{1}{2}\gamma(z_{n+1} - z_n) + 1\right] + \right. \\
&\left. + e^{-\gamma(z_n + z_{n-1})}(z_n - z_{n-1})\left[\tfrac{1}{2}\gamma(z_n - z_{n-1}) - 1\right]\right\}, \\
\frac{d^2 y_n}{dt^2} &= S(y_{n+1} - 2y_n + y_{n-1}) + S\rho\left\{e^{-\gamma(y_{n+1}+y_n)}(y_{n+1} - y_n)\left[\tfrac{1}{2}\gamma(y_{n+1} - y_n) + 1\right] + \right. \\
&\left. + e^{-\gamma(y_n + y_{n-1})}(y_n - y_{n-1})\left[\tfrac{1}{2}\gamma(y_n - y_{n-1}) - 1\right]\right\} - 2\sqrt{2}e^{-\sqrt{2}y_n}\left[1 - e^{-\sqrt{2}y_n}\right],
\end{aligned} \tag{1}$$

Here $S = \frac{K}{d\alpha^2}$, $\gamma = \frac{\alpha}{a}$ are dimensionless parameters; K is the constant which characterizes interaction between pairs of bases along the chain; ρ is the parameter which characterizes the nonlinearity in the system; α is the parameter which characterizes a decrease of stacking interaction.

2. Long-wavelength limit

Considering a case of the long-wavelength limit (this is a case of low frequencies), one assumes that a value of $1/a$ is essentially smaller than to the wave length. Transformation of the system (1) to corresponding distributed system can be made by use of the following approximate relations:

$$z_{i+1} - z_i \approx a\frac{dz}{dx},\ y_{i+1} - y_i \approx a\frac{dy}{dx};\ y_{i+1} - 2y_i + y_{i-1} \approx a^2\frac{d^2y}{dx^2},\ z_{i+1} - 2z_i + z_{i-1} \approx a^2\frac{d^2z}{dx^2} \tag{2}$$

Besides, the following approximations are used: $y_i \sim y(x)$; $y_{i+1} \sim y(x)$, $z_i \sim z(x)$; $z_{i+1} \sim z(x)$. Taking into account all mentioned approximations, one obtains from the system (1) the following equations of the long-wavelength limit:

$$\begin{cases} \frac{d^2z}{dt^2} = \beta\frac{d^2z}{dx^2} + \sigma e^{-2\gamma z}\left(\frac{dz}{dx}\right)^2 \\ \frac{d^2y}{dt^2} = \beta\frac{d^2y}{dx^2} - 2\sqrt{2}e^{-\sqrt{2}y}\left[1 - e^{-\sqrt{2}y}\right] + \sigma e^{-2\gamma y}\left(\frac{dy}{dx}\right)^2 \end{cases} \tag{3}$$

where $\beta = a^2 S,\ \sigma = \gamma\beta\rho,\ \gamma = \frac{\alpha}{a}$ are dimensionless parameters.

Traveling waves in the form $z = \Phi_1(\varphi);\ y = \Phi_2(\varphi)$, where $\varphi = kx - \omega t$ is the phase of the wave, are analyzed. For these solutions one obtains from equations (3) the ODE system. Assuming that values of variables Φ_1 and Φ_2 are not large, one expands exponents to Tailor series, saving then nonlinear terms up to third degree on $\Phi_1, \frac{d\Phi_1}{d\varphi}$ and $\Phi_2, \frac{d\Phi_2}{d\varphi}$. One has

$$\begin{cases} \frac{d^2\Phi_1}{d\varphi^2}(\omega^2 - \beta k^2) - \sigma k^2\left(\frac{d\Phi_1}{d\varphi}\right)^2(1 - 2\gamma\Phi_1) = 0 \\ \frac{d^2\Phi_2}{d\varphi^2}(\omega^2 - \beta k^2) + 4\Phi_2 - 6\sqrt{2}{\Phi_2}^2 + \frac{28}{3}{\Phi_2}^3 - \sigma k^2\left(\frac{d\Phi_2}{d\varphi}\right)^2(1 - 2\gamma\Phi_2) = 0 \end{cases} \tag{4}$$

Analysis of the first equation of the system (4), which is not presented here, shows that corresponding motions are unbounded. It is a consequence of the fact that the coordinate Φ_1 describes motions of the center of masses for which any limitations are absent. So, only the second equation of the system (4) will be analyzed. It can conclude that solitary waves in the long-wavelength limit are absent because we have only the single equilibrium position, namely, $\Phi_2 = 0$. We introduce to the second equation of the system (4) the small parameter ε which characterizes a smallness of nonlinear terms in the system under consideration. One introduces also the new independent variable τ by the following relation:

$$\varphi = \mu\tau. \tag{5}$$

Here μ is some constant. It will be determined in process of construction of the solution which must be 2π- periodic by τ. Introducing the new independent variable τ instead of the argument φ, one obtains from the second equation of the system (4) the following equation (here "prime" means derivation by the new independent variable τ):

$${\Phi_2}''_\tau(\omega^2 - \beta k^2) + 4\mu^2\Phi_2 + \varepsilon\left[-6\sqrt{2}{\Phi_2}^2\mu^2 + \frac{28}{3}\mu^2{\Phi_2}^3 - \sigma k^2{\Phi_2}'^2_\tau(1 - 2\gamma\Phi_2)\right] = 0 \tag{6}$$

In correspondence with the small parameter method a solution of the equation (6) is determined in power series with respect to the small parameter ε,

$$\Phi_2 = \Phi_{20} + \varepsilon\Phi_{21} + \cdots;\ \mu = \mu_0 + \varepsilon\mu_1 + \cdots \tag{7}$$

Introducing the power series (7) to the equation (6), one has

$$\begin{aligned} &({\Phi_2}''_0 + \varepsilon{\Phi_2}''_1 + \cdots)(\omega^2 - \beta k^2) + 2(\mu_0 + \varepsilon\mu_1 + \cdots)^2(\Phi_{20} + \varepsilon\Phi_{21} + \cdots) + \\ &+\varepsilon\left[\left(-6\sqrt{2}(\Phi_{20} + \varepsilon\Phi_{21} + \cdots)^2 + \frac{28}{3}(\Phi_{20} + \varepsilon\Phi_{21} + \cdots)^3\right)(\mu_0 + \varepsilon\mu_1 + \cdots)^2 - \right. \\ &\left. -\sigma k^2({\Phi_2}'_0 + \varepsilon{\Phi_2}'_1 + \cdots)^2(1 - 2\gamma(\Phi_{20} + \varepsilon\Phi_{21} + \cdots))\right] = 0 \end{aligned} \tag{8}$$

Then equations in the first two approximations by the small parameter are considered. In each

approximation values of μ_0 and μ_1 are chosen in order that to eliminate secular terms in solutions. Besides, taking into account the fact that the system is conservative, it can use the additional condition: $\Phi_2'(0) = 0$. We do not present here details of standard transformations; one writes a solution of the equation (8), returning to the argument φ:

$$\Phi_2 = a_0 \cos\left(\frac{\varphi}{\mu}\right) - \frac{\varepsilon}{(\omega^2-\beta k^2)}\left[\frac{a_0^2}{\theta}\left(3\sqrt{2}\mu_0^2 + \frac{\sigma k^2}{2}\right) + \frac{a_0^2\left(3\sqrt{2}\mu_0^2 - \frac{\sigma k^2}{2}\right)}{(\theta-4)}\cos\left(2\frac{\varphi}{\mu}\right) - \right.$$
$$\left. - \frac{a_0^3}{(\theta-9)}\cos\left(3\frac{\varphi}{\mu}\right)\left[\frac{\gamma\sigma k^2}{2} - \frac{7}{3}\mu_0^2\right]\right] + O(\varepsilon^2) \qquad (9)$$

where $\mu = \mu_0 + \varepsilon\frac{a_0^2\left(7\mu_0^2 + \frac{1}{2}\gamma\sigma k^2\right)}{4\mu_0}$, $\theta = \frac{2\mu_0^2}{\omega^2-\beta k^2}$, $\mu_0 = \frac{\sqrt{\omega^2-\beta k^2}}{\sqrt{2}}$.

It can see that a term of the first order by ε is small with respect to the main term of expansion if the wave amplitude a_0 is relatively small. To estimate an exactness of the obtained analytical solution we compare it with numerical solution of the second equation (4), which is obtained by the Runge-Kutta method of the 4-th order. The comparison is made for initial solutions which are common both for analytical solution, and numerical one. These initial conditions are chosen as $\Phi_2(0) = 0.049$, $\Phi_2'(0) = 0$. The system parameters are the following: $a = 4\ A^{-1}$, K = 0.01 eV/A^2, ρ = 3, α = 0.8 A^{-1} [4]. Besides, the connection parameter is chosen as S = 0.0119; other parameters are: γ = 0.2, σ = 0.14, ω = 1.12, F = 0.05, ε = 1. It can see a good coincidence of the analytical and numerical solutions (Fig.2).

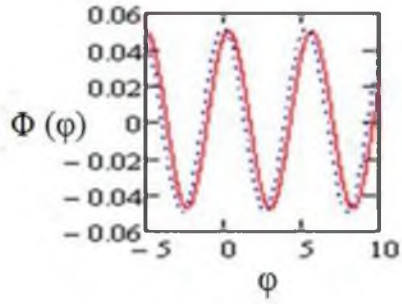


Figure 2. Comparison of analytical and numerical solutions for the long-wavelength limit. Solid line corresponds to the numerical solution; points correspond to the analytical solution.

2.1. Dispersion relation for the long-wavelength limit

Dispersion relation for the long-wavelength limit in the PBD model can be obtained by the small parameter method. For it the second equation of the system (4) is rewritten as

$$\frac{d^2\Phi_2}{d\varphi^2}(\omega^2 - \beta k^2) + 4\Phi_2 - 6\sqrt{2}{\Phi_2}^2 + \frac{28}{3}{\Phi_2}^3 - \sigma k^2\left(\frac{d\Phi_2}{d\varphi}\right)^2(1 - 2\gamma\Phi_2) = 0 \qquad (10)$$

Then nonlinear terms in the equation (10) must be multiply to the small parameter ε, and the power series by ε are used:

$$\Phi_2 = \Phi_{2_0} + \varepsilon\Phi_{2_1} + \cdots \qquad \omega^2 = \omega^2(k) = \omega_0^2 + \varepsilon\omega_1^2 + \cdots \qquad (11)$$

Introducing expansions (11) to the equation (10) and comparing terms of the same orders by ε, one has the following:

ε^0:

$$\Phi''_{20}(\omega_0{}^2 - \beta k^2) + 4\Phi_{20} = 0 \tag{12}$$

ε^1:

$$\Phi''_{21}(\omega_0{}^2 - \beta k^2) + 4\Phi_{21} = -\omega_1^2\Phi''_{20} + 6\sqrt{2}\Phi_{20}{}^2 - \\ -\frac{28}{3}\Phi_{20}{}^3 + \sigma k^2\Phi'_{20}{}^2(1 - 2\gamma\Phi_{20}) = 0 \tag{13}$$

It can obtain the 2π –periodic solution if the following conditions of periodicity are satisfied:

$$\omega_0^2 = 4 + \beta k^2;\ \ \omega_1^2 B - 7B^3 - \frac{1}{2}\sigma k^2\gamma B^3 = 0 \tag{14}$$

Here a solution of the zero approximation is presented as $\Phi_{20} = B\cos(\varphi)$.

As a result, using the relations (14) and the expansion (11), one obtains the dispersion relation, which describes the dependence of the frequency ω on the amplitude B as

$$\omega^2 = 4 + \beta k^2 + \varepsilon\left[7B^2 + \frac{1}{2}\sigma k^2\gamma B^2\right] \tag{15}$$

3. Anti-phase vibration modes

The other limit case is also considered here, namely, the high-frequency anti-phase vibration modes, which represent **standing waves.**

1) One of them describes unidirectional motions of the upper and lower disks of the DNA molecule, where these emotions are anti-phase with respect to motions of neighboring particles of the chain. So, one has $u_i = v_i$; it corresponds to the following relations:

$$z_i = z_i(t), y_i = 0.$$
$$-z_{i-1} = z_i, -z_{i+1} = z_i \tag{16}$$

2) $u_i = -v_i$; it corresponds to the following relations: The second vibration mode describes opposite motions of the upper and lower disks, that is,

$$y_i = y_i(t), z_i = 0; \quad -y_{i-1} = y_i, -y_{i+1} = y_i \tag{17}$$

The **anti-phase mode 1)** is described by the following ODE which is obtained from the system (1) under relations (16):

$$\frac{d^2z}{dt^2} + z[4S(1+\rho)] - z^2 4S\rho\gamma = 0 \tag{18}$$

The small parameter method is used here to determine solutions of the equations (20) near the trivial equilibrium position. Introducing the new independent variable ψ, we will find the solution which is 2π -periodic by ψ. The following transformation is used:

$$t = \nu_1\psi, \tag{19}$$

where ν_1 is some constant which will be determined by construction of the periodic solution. One has

the following equation instead of the equation (18):

$$\frac{d^2z}{d\psi^2} + zv_1^2[4S(1+\rho)] - 4\varepsilon v_1^2 S\rho\gamma z^2 = 0 \tag{20}$$

Here the small parameter ε characterizes a smallness of nonlinear terms with respect to linear ones. A solution of the equation (20) is determined in power series with respect to the small parameter ε, namely,

$$z = z_0 + \varepsilon z_1 + \cdots \qquad v_1 = v_{1_0} + \varepsilon v_{1_1} + \cdots \tag{21}$$

We do not present here details of standard construction; one writes a solution of the equation (21), returning to the argument φ, as

$$z = G\cos\left(\frac{t}{v_{1_0}}\right) + \varepsilon\left[\frac{2S\rho\gamma v_{1_0}^3 G^2}{\Omega_1} + \frac{2S\rho\gamma v_{1_0}^2}{(\Omega_1-4)}G^2\cos\left(\frac{2t}{v_{1_0}}\right)\right] + O(\varepsilon^2) \tag{22}$$

где $v_{1_0} = \frac{1}{\sqrt{[4S(1+\rho)]}}$, $v_{1_0} = 0$.

The expansion (22) is uniform; it can see that a term of the first order by ε is small with respect to the main term of expansion if the wave amplitude G is relatively small.

For the **anti-phase mode of the form 2)** one obtains the following ODE from the system (1):

$$\frac{d^2y}{dt^2} = 4Sy[-1 + \rho(\gamma y - 1)] + 2\sqrt{2}e^{-\sqrt{2}y}\left(e^{-\sqrt{2}y} - 1\right) \tag{23}$$

Expanding exponents to Tailor series and saving nonlinear terms up to third degree on y and $\frac{dy}{dt}$, one has

$$\frac{d^2y}{dt^2} + y(4[S(1+\rho)+1]) - y^2(6\sqrt{2} + 4S\rho\gamma) + \frac{28}{3}y^3 = 0 \tag{24}$$

Repeating standard transforms of the small parameter method, one obtains, as a result, the following solution of the equation (24):

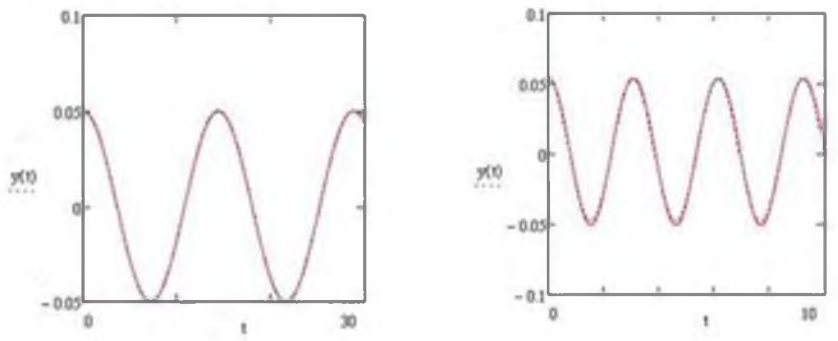
$$y = F\cos\left(\frac{t}{v_2}\right) + \varepsilon\left[\frac{F^2 v_{2_0}^2(3\sqrt{2}+2S\rho\gamma)}{\eta} + \right.$$
$$\left. + \cos\left(\frac{2t}{v_2}\right)\frac{F^2(3\sqrt{2}+2S\rho\gamma)v_{2_0}^2}{(\eta-4)} - \frac{7v_{2_0}^2F^2}{3(\eta-9)}\cos\left(\frac{3t}{v_2}\right)\right] + O(\varepsilon^2), \tag{25}$$

where $v_2 = v_{2_0} - \varepsilon\frac{7v_{2_0}F^2}{2[4+4S(1+\rho)]}$, $v_{2_0} = \frac{1}{\sqrt{4+4S(1+\rho)}}$.

It can see that a term of the first order by ε is small with respect to the main term of expansion if the amplitude F is relatively small. The expansion (25) is uniform one.

Comparing two obtained anti-phase vibration modes, we use the same parameters as in the long-wavelength case (Section 2). Here the anti-phase mode 2) has a frequency $\nu = 2.292$, and the anti-phase mode 1) has a frequency $\nu = 0.488$. So, namely the mode 2) has the higher frequency.

Analytical solutions (22) and (28) were compared with numerical solutions of equations (18) and (24), obtained by the Runge-Kutta method of the 4-th order. Initial solutions of the analytical and numerical solutions are the same, namely, $z(0) = 0.049, z'(0) = 0$; the same initial values are used for the variable y. The system parameters are the same as in the long-wavelength approximation. We can see that diagrams of these solutions coincide. It shows a good exactness of the approximate analytical solutions.



a) b)

Figure 3. Diagrams of analytical and numerical solutions describing the anti-phase vibration modes. Solid line corresponds to the numerical simulation; dotted one – to the analytical solution. Plot in Fig. 2,a) is obtained for the anti-phase mode 1); plot in Fig. 2.б) is obtained for the anti-phase mode 2).

4. Stability of the localized standing waves

Localized standing waves are excited by initial displacement, or velocity of some chosen disk in the PBD model. Stability of the solution is analyzed by the numerical-analytical approach which is a consequence of the known Lyapunov definition of stability [8]. Namely, values of kinetic energies (or velocities) of the chosen disk and neighboring elements are compared. We fix the instability if more than 10 percent of the initial kinetic energy passes to these neighboring discs. Calculations are made at points on some chosen mesh of the system parameter space. Calculations are conducted as long as boundaries of stability/ instability regions (in a chosen scale) on the system parameter space are variable. This is the principal criterion for the choice of the calculation time T.

Results of calculations are presented in Fig. 3, where boundaries of stability/ instability regions in the system configuration space are shown. Here $\alpha = 0.65$ $\gamma = 0.577$. The stability regions are situated from the left of the boundaries.

Conclusions

Traveling and standing waves in the model by Peyrard-Bishop- Dauxois (PBD model), which describes the dynamics of the DNA molecule, are considered. Traveling waves are constructed in the long-wavelength limit by the small parameter method; here the small parameter characterizes a smallness of the nonlinear terms in the PBD model. The most high-frequency modes, namely, anti-phase modes, are constructed also by the small parameter method. Stability of standing localized modes is analyzed. Checking numerical simulation shows good exactness of the obtained approximate analytical solutions.

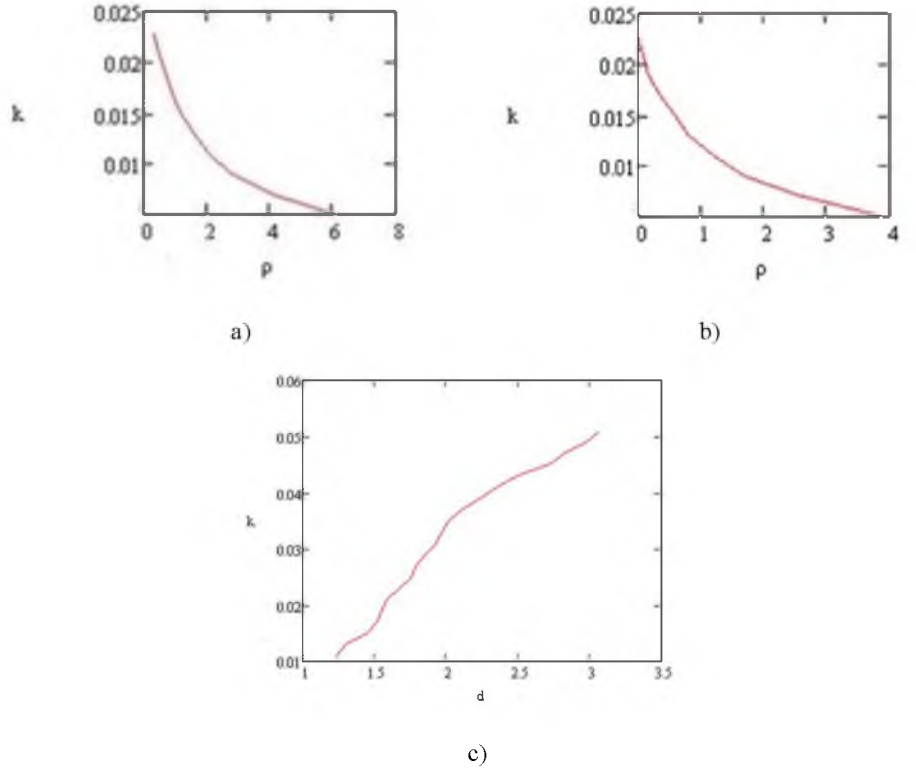


Figure 3. Boundaries of the stability/ instability regions in the system (1) space of parameters. Figs. 3a,b – boundaries in the place (k, ρ) for d=0.9 (Fig.3a) and d=0.33 (Fig.3b); Fig. 3c – boundaries in the place (k, d) for ρ=0.5.

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