STUDY ON LINEAR STABILITY OF REACTION-DIFFUSION SYSTEM WITH OREGONATOR REACTION MODEL

A THESIS SUBMITTED IN PARTIAL

FULFILMENT OF THE REQUIREMENTS FOR

THE DEGREE OF

MASTER OF TECHNOLOGY

BY

KUNDAN KUMAR

(20102022)

TO THE

DEPARTMENT OF CHEMICAL ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY KANPUR

MAY 2022

Certificate

It is certified that the work contained in the thesis titled " **STUDY ON LINEAR STABILITY OF REACTION DIFFUSION SYSTEM WITH OREGONATOR REACTION MODEL**" by "Kundan Kumar" has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

Raghvendra Singh

Signature of Supervisor
Professor: Dr.Raghvendra Singh
Department: CHE
IIT kanpur

DECLARATION

This is to certify that thesis titled "STUDY ON LINEAR STABILITY OF REACTION DIFFUSION SYSTEM WITH OREGONATOR REACTION MODEL" has been authored by me. It presents the research conducted by me under the supervision of Dr.Raghvendra Singh.To the best of my knowledge, it is an original work, both in terms of research content and narrative, and has not been submitted elsewhere, in part or in full, for a degree. Further, due credit has been attributed to the relevant state-of-the-art and collaborations (if any) with appropriate citations and acknowledgements, in line with established norms and practices.

Kundan

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ABSTRACT

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Thesis Title: Study on the linear stability of the reaction-diffusion system with Oregonator model as the reaction term**.**

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Month and year of Thesis Submission: April 2022

Oscillating reactions like the Belousov-Zhabotinsky(BZ) reaction are far from equilibrium and the concentration of species oscillates with time and/or position. The study of instability in reaction-diffusion systems with oscillating reactions helps to understand various biological patterning phenomena like pattern formation in cell division, embryo development and skin color patterns. The focus of the current study is to do the linear stability analysis of the reaction-diffusion system with the reaction term approximated by the Oregonator model. The Oregonator model is a simplified reaction mechanism for Belousov Zhabotinsky reaction. The behaviour of the system for small perturbations was studied by plotting the variation of growth rate with wavenumber for different initial conditions. The value of wavenumber at which the system becomes unstable, that is growth rate becomes positive was noted. The variation of steady-state with D_a was also studied in the later part.

ACKNOWLEDGEMENT

I want to express my sincere gratitude to my thesis supervisor, Prof. Raghvendra Singh, for his invaluable suggestions in shaping and giving the right direction to the research topic through his regular zoom meetings, discussion and continuous motivation. I am obliged to him for bringing out the best in me and boosting my confidence. I would like to thank my friends and family for their constant love and support. I would also like to thank IIT Kanpur for providing me necessary resources for completing my thesis.

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INTRODUCTION

Generally, in a reaction, we can observe that the concentration of reactants and products monotonically reaches an equilibrium value as time progresses. But in oscillating reactions like Belousov Zhabotinsky (BZ) reaction, some component's concentration oscillates with time and position until reactants are entirely consumed. These oscillating reactions have applications in spatial organization and pattern formation in biological systems like cell division, embryo development and color patterns on animal skins. This similarity is because the governing mathematical equations are similar.[1] Some other applications of oscillating reactions are designing self-oscillating gels and in the analytical determination of various organic and inorganic compounds.[2, 3].

Oscillating reactions

Some examples of oscillating reactions are as follows-

i. Belousov-Zhabotinsky(BZ) reaction-

Oscillations can be observed by the change in color/electrode potential of the solution. The color of the solution oscillates between yellow and clear. The overall reaction is given by[4]-

$BrO^{3-} + 3CH_2(COOH)_2 + 2H^+ \rightarrow 3CO_2 + 2\ BrCH(COOH)_2 + 4H_2O$

ii. Bray–Liebhafsky reaction-
This is a redox reaction where hydrogen peroxide oxidizes and reduces the iodine compounds in an acidic solution. [5]

$5H_2O_2 + 2IO^{3-} + 2H^+ \rightarrow I_2 + 5O_2 + 6H_2O$

$5H_2O2 + I_2 \rightarrow 2IO^{3-} + 2H^+ + 4H_2O$

Overall the reaction is given by

$2H_2O2 \rightarrow 2H_2O + O_2$.

iii. Briggs-Rausher reaction-

It is the combination of the BZ reaction and the Bray-Liebhafsky reaction. This reaction is acidic oxidation of malonic acid by the mixture of hydrogen peroxide and iodate in the presence of a manganous catalyst, followed by starch addition. The color of the solution oscillates between clear, amber and blue. The final solution is of dark blue-black color.[6]

The overall reaction is given by[6, 7]

$IO_3^- + 2\ H_2O_2 + CH_2(CO_2H)_2 + H^+ \rightarrow ICH(CO_2H)_2 + 2\ O_2 + 3\ H_2O$.

There is no specific set of conditions that is sufficient to determine whether a reaction is oscillatory. Still, there are some common traits between different oscillating reactions like the system is far from equilibrium, nonlinear dynamics, autocatalysis, and bistability [8]. Autocatalysis is present in almost all oscillators. Autocatalytic reactions are those reactions in which one of the products of the reaction acts as a catalyst.

Reaction mechanism of BZ reaction

The reaction mechanism was first suggested by Field, Koros & Noyes (FKN). The detailed mechanism is very complex and includes many elementary steps[1]. The reaction mechanism can be understood in three parts[4, 9]-

Part 1. Reduction of bromate to bromine.

$BrO^{3-} + 5Br^- + 6H^+ \rightarrow 3Br_2 + 3H_2O$

Part 2. Reduction of Bromate to Hypobromous acid autocatalytically with oxidation of metal ion(Ce^{3+}), where bromous acid($HBrO_2$) acts as a catalyst.

$BrO^{3-} + 4Ce^{3+} + 5H^+ \rightarrow HOBr + 4Ce^{4+} + 2H_2O$

Part 3. Oxidation of Bromomalonic and malonic acid with Ce^{4+}.The organic acids are brominated with the help of Br2 and HOBr formed in part (1) and (2).

$4Ce^{4+} + BrCH(COOH)2 + H2O + HOBr \rightarrow 4Ce^{3+} + 3CO_2 + 6H^+ + 2Br^-$

$6Ce^{4+} + CH2(COOH)2 + H2O + HOBr \rightarrow 6Ce^{3+} + 3CO_2 + 7H^+ + Br^-$

Other metal ions like Ferrion(iron complexed with orthophenanthroline) can also be used and it shows a color change from brick red to blue.[9].

Oregonator Model

Oregonator is a simple reduced model for the BZ reaction mechanism and the results from this model quite closely agree with the experiments. [10].The reaction mechanism is reduced to five elementary reactions, which are [11]-

1. A + Y → X + P $r_1 = k_1AY$
2. X + Y → 2P $r_2 = k_2XY$
3. A + X → 2X + 2Z $r_3 = k_3AX$
4. X + X → A + P $r_4 = k_4X^2$
5. B + Z →1/2*f Y $r_5 = k_5BZ$

Where A =BrO^{3-}, B=$CH_2(COOH)_2$,P=HOBr/BrCH$(COOH)_2$, X=$HBrO_2$, Y=Br^-, Z= Ce^{4+}

$$\frac{dX}{dt} = k_1AY - k_2XY + k_3AX - 2k_4X^2$$

$$\frac{dY}{dt} = -k_1AY - k_2XY + \frac{1}{2}fk_5BZ$$

$$\frac{dZ}{dt} = 2k_3AX - k_5BZ$$

In dimensionless form above three ODEs can be written as-

$$p_x\frac{dx}{dt} = x(1-x) - y(x-q) \quad (1)$$

$$p_y\frac{dy}{dt} = bgz - y(x+q) \quad (2)$$

$$\frac{dz}{dt} = x - bz \quad (3)$$

where x, y, z are the dimensionless concentration with respect to some arbitrary constants (mol/L) of $HBrO_2$, $Br^-$and Ce^{4+} respectively. q, b, g, p_x, p_y are constants and their value depends upon the total concentration of species, arbitrary constants and various rate constants.[10].

Further, if $p_y = 0$ in equation (2) then the system of equations is reduced to the following coupled ODEs-

$$p_x \frac{dx}{dt} = x(1-x) - fz(x-q)/(x+q) \tag{4}$$

where f=bg

$$\frac{dz}{dt} = x - bz \tag{5}$$

Equations (4) and (5) are used for stability analysis in this thesis. Based on assumptions, there can be various other reaction models. Some of them are-model K, model of Schmidt and Ortoleva.[10]In this thesis, only Oregonator model is used.

Instability

Reynolds studied the instability of flow in a pipe through dye experiment. He discovered that below a critical dimensionless number (Re=ρvd/μ), flow is laminar and above it becomes unstable and changes to turbulence. It is believed that this experiment motivated the study of stability analysis of fluid flow.[12].An equilibrium or steady solution is said to be stable if perturbations introduced in the system decay or remain the same with time.[13] There are various methods to study stability like linear analysis, graphical method, nonlinear analysis, computational and numerical methods.

In this writing, the linear stability analysis is used to study the onset of instability in the diffusion-reaction system.

Linear stability analysis-

In linear stability analysis, the governing equations are linearized about the fixed or equilibrium points.

Consider a system $\frac{dx}{dt} = g(x)$

For fixed points $\frac{dx}{dt} = g(x*) = 0$ where x* is a fixed point.

Let *x(t)=x*+η(t)* where η is perturbation and $\eta \ll 1$.

$$\frac{d\eta}{dt} = g(x* + \eta)$$

Taylor expanding about x*

$$g(x^*+\eta) = g(x*) + \eta g'(x*) + \frac{\eta^2}{2!} g''(x*) + \cdots$$

Ignoring the nonlinear terms as $\eta \ll 1$.

$$\frac{d\eta}{dt} = g'(x*)\eta$$

A general solution is of the form exp[$g'(x*)\, t$] so the solution will decay or grow according to the sign of g'(x*). If g'(x*) is negative, then the perturbations will decay with time, and if it's positive, it will grow. If g'(x*) =0, then linear stability cannot be used. Graphical method can be used to determine stability in such cases, or higher order terms have to be included.

Similarly for a system of coupled ODEs

$$\frac{dx}{dt} = \boldsymbol{g}(\boldsymbol{x}) \quad \text{where } \boldsymbol{x} = (x_1, x_2, x_3 \ldots x_n)$$

for **x**(t)=**x***+**η**(t) and doing Taylor expansion and ignoring non-linear terms we get

$$\frac{d\boldsymbol{\eta}}{dt} = \boldsymbol{J}(x*)\boldsymbol{\eta} \text{ where } \boldsymbol{J} \text{ is Jacobian of } \boldsymbol{g} \text{ and } J(i,j) = \frac{\partial g_i}{\partial xj}$$

Let η is of the form exp(st) where s is the growth rate, then the above equation has a non-trivial solution if [14]

$$det(\boldsymbol{J} - s\boldsymbol{I}) = 0$$

This will give the characteristic equation and if the real part of **s** is negative, i.e., the eigenvalues of *J*, then the perturbations will decay with time and if Re(s) is positive, it will grow. Initial conditions are not required to predict the growth/decay of perturbations as clear from the above analysis. So instead of solving the IVP (Initial value problem), we solve the EVP(eigenvalue problem) to know the asymptotic stability. Also, in many cases, initial conditions are not known completely.

Method of Normal modes-

In normal modes the perturbations,η is taken in the form of *f(**x**)exp(st)* where s is the growth rate and it can be complex in general and the sign of s decides the stability. After substituting this form we get a steady-state solution and perturbation equations.This method cannot predict the initial transient growth that can be there in the system[15]. In this thesis, perturbations of $\varepsilon exp(i\kappa x + \beta t)$ normal form have been taken, where κ is the wavenumber and β is the growth rate.

Reaction-Diffusion system

This system was first used by Alan Turing to study pattern formations.

$$\frac{\partial C_i}{\partial t} = \mathrm{D}_i \nabla^2 C_i + f_i(C_1, C_2, C_3 \ldots C_n)$$

Where $f(C_i)$ is the reaction term and C_i is the concentration. These systems can produce patterns from a homogeneous state because of inherent disturbances present in the system. The RD(reaction-diffusion) model can explain many biological patterning phenomena[16]. In this thesis, Belousov Zhabotinsky(BZ) reaction and Oregonator model for the reduced reaction mechanism have been used for f_i term in RD system.

$$\frac{\partial a}{\partial t} = \frac{D_a}{d^2} \nabla^2 a + \frac{\left[a - a^2 - \frac{fb\,(a-q)}{a+q}\right]}{e} \tag{6}$$

$$\frac{\partial b}{\partial t} = \frac{D_b}{d^2} \nabla^2 b + (a - b) \tag{7}$$

Let $a = a_s + \varepsilon exp(i\kappa x + \beta t)$ and $b = b_s + \varepsilon exp(i\kappa x + \beta t)$

Where a_s and b_s are steady-state values, κ is the wavenumber of disturbance in the x-direction and β is the growth rate. $\varepsilon \ll 1$, so ignoring the terms of order $O(\varepsilon^2)$ and higher.

Substitute a and b in equations (6) and (7)

Eqn 6 becomes-

$$\varepsilon\beta \exp(i\kappa x + \beta t) = \frac{D_a}{d^2} * [\nabla^2 a_s - \varepsilon\kappa^2 \exp(i\kappa x + \beta t) +$$

$$a_s + \varepsilon \exp(i\kappa x + \beta t) - (a_s^2 + 2a_s\varepsilon \exp(i\kappa x + \beta t) + \varepsilon^2 \exp 2 * (i\kappa x + \beta t)) -$$

$$\frac{f\,[b_s a_s + b_s\varepsilon \exp(i\kappa x + \beta t) + a_s\varepsilon \exp(i\kappa x + \beta t) + \varepsilon^2 \exp 2(i\kappa x + \beta t) - q b_s - q\varepsilon \exp(i\kappa x + \beta t)]}{e(a_s + \varepsilon \exp(i\kappa x + \beta t) + q)}$$

Ignoring $O(\varepsilon^2)$ terms and using the expansion $\frac{1}{1+x} = 1 - x + x^2 - x^3 + \cdots$

The steady state solution is

$$\frac{D_a}{d^2} \nabla^2 a_s + \frac{\left[a_s - a_s^2 - \frac{f b_s (a_s - q)}{a_s + q}\right]}{e} = 0 \tag{8}$$

perturbations term-

$$\beta = -\frac{\kappa^2 D_a}{d^2} + \frac{1-2a_s}{e} - \frac{f(a_s+b_s-q)}{e(a_s+q)} - \frac{fb_s(a_s-q)}{(as+q)^2} \tag{9}$$

Similarly, after substituting a and b, equation-7 becomes

$$\varepsilon\beta\exp(i\kappa x + \beta t) = \frac{D_b}{d^2}(\nabla^2 b_s - \varepsilon\kappa^2\exp(i\kappa x + \beta t)) + a_s + \varepsilon\exp(i\kappa x + \beta t) - b_s - \varepsilon\exp(i\kappa x + \beta t)$$

Separating the steady and perturbed terms, the steady-state solution is

$$\frac{D_b}{d^2}\nabla^2 b_s + (a_s - b_s) = 0 \tag{10}$$

and perturbation term

$$\beta = -\frac{k^2 D_b}{d^2} \tag{11}$$

let $\frac{dy_1}{dx} = y_2$ (12)

and $\frac{dy_3}{dx} = y_4$ (13)

where $y_1=a_s$ and $y_3=b_s$, then equations (8) and (10) becomes

$$\frac{D_a}{d^2}\frac{dy_2}{dx} + \frac{\left[y_1 - y_1^2 - \frac{fy_3(y_1-q)}{y_1+q}\right]}{e} = 0 \tag{14}$$

$$\frac{D_b}{d^2}\frac{dy_4}{dx} + y_1 - y_3 = 0 \tag{15}$$

Equations 12-15 with the initial boundary condition y0= $[y_1, y_2, y_3, y_4]$ at x=0 are solved in MATLAB using ode45 solver. The value of parameters taken are D_a=1, D_b=0.6, d=0.2, f=1.4, q=0.002, e=0.01.

After getting a_s and b_s, growth rate vs. wavenumber (β vs. κ) is plotted using equation -9 for different x to check whether the perturbations decay or grow based on the sign of β.

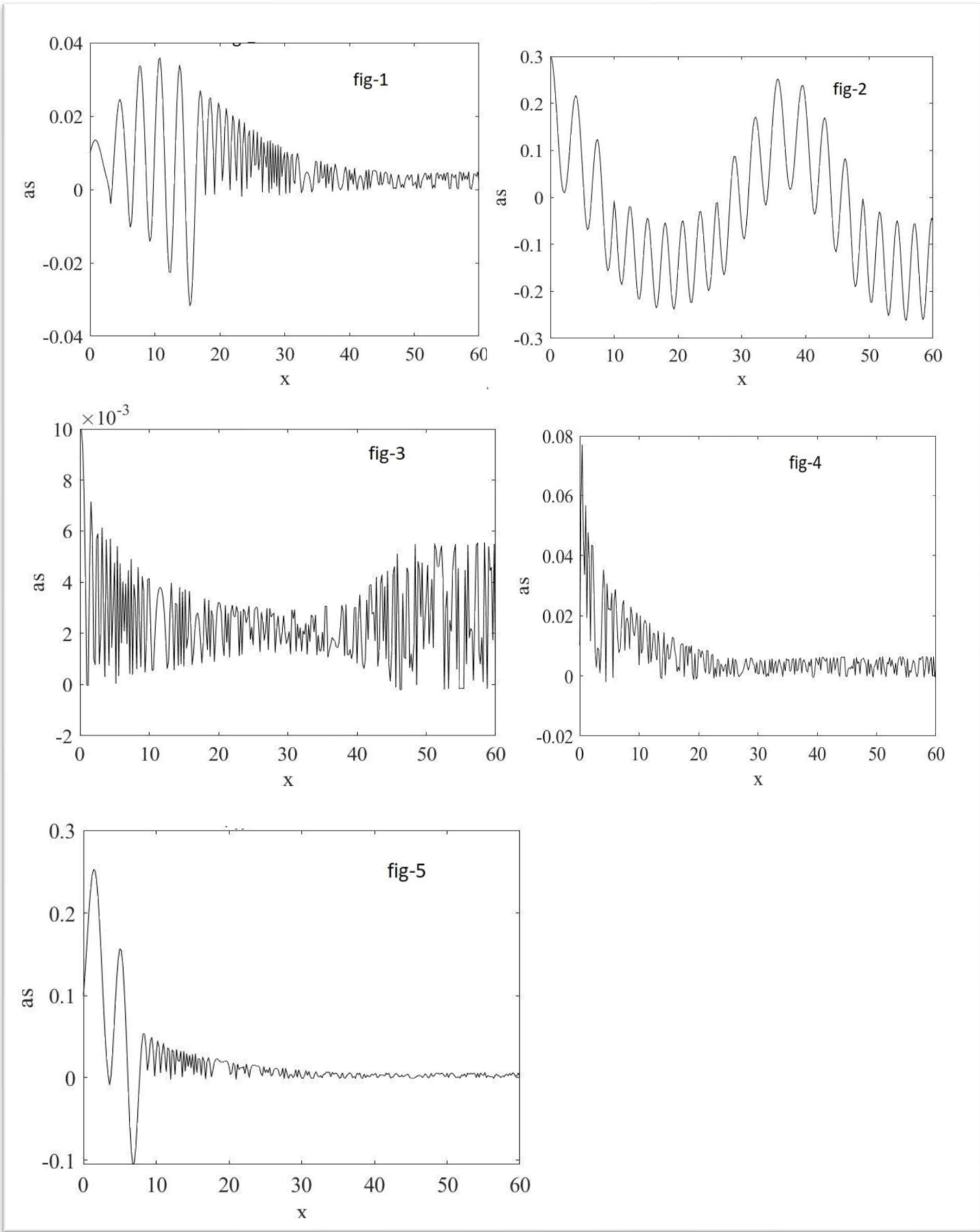
Also, D_a is varied, keeping other parameters constant to see the change in steady-state with diffusivity.

Pattern formation

In nature, we can find patterns almost everywhere for example -sand dunes in the desert and color patterns on animal skin like zebrafish, squirrels and tigers.[17, 18].There is a pattern in electrical signal of beating heart, hair follicles [9].Many developmental biological phenomenon like tooth formation, digit formation during limb development, embryo development also shows patterns or structure.[19]A recent study shows the Turing pattern is also observed in atomically thin Bismuth[20]. The patterns can be in the form of waves, spirals, and stationary patterns like stripes, dots[1] depending upon the values of parameters. These patterns can be studied with instability analysis of reaction-diffusion(RD) system.[21] There are other models to study the patterns but very few of them are as good as reaction-diffusion model. Turing showed how an initially homogeneous system leads to pattern formation because of instability due to perturbations. Because of the complex nature of biological phenomena and heterogeneity, Turing's instability, which assumes a homogenous medium, does not give a complete understanding of biological patterns.[18, 22] .The patterning phenomenon is very diverse. It can be external, for example, color patterns, or internal, like calcium waves in cells. So it is still challenging to describe the patterning phenomenon in biology exactly. The pattern formed in one system can be found in other systems also because of mathematical similarity of governing equations. So understanding patterns in oscillating reactions can give insights to dynamics of pattern of other systems also.

RESULT AND DISCUSSION

Result -1. Steady states for different values of y0



The steady state(as) is plotted using MATLAB for different values of y0 keeping other parameters constant which are - as D_a=1, D_b=0.6, d=0.2, f=1.4, q=0.002, e=0.01.

1. In fig-1, y0= [0.01,0.007,0.01, -0.000110] and the amplitude of oscillations increases till x=15(approximately) after that it decreases continuously.

2. In fig- 2, y0= [0.3,0.007,0.01, -0.000110] and there is sustained oscillation.

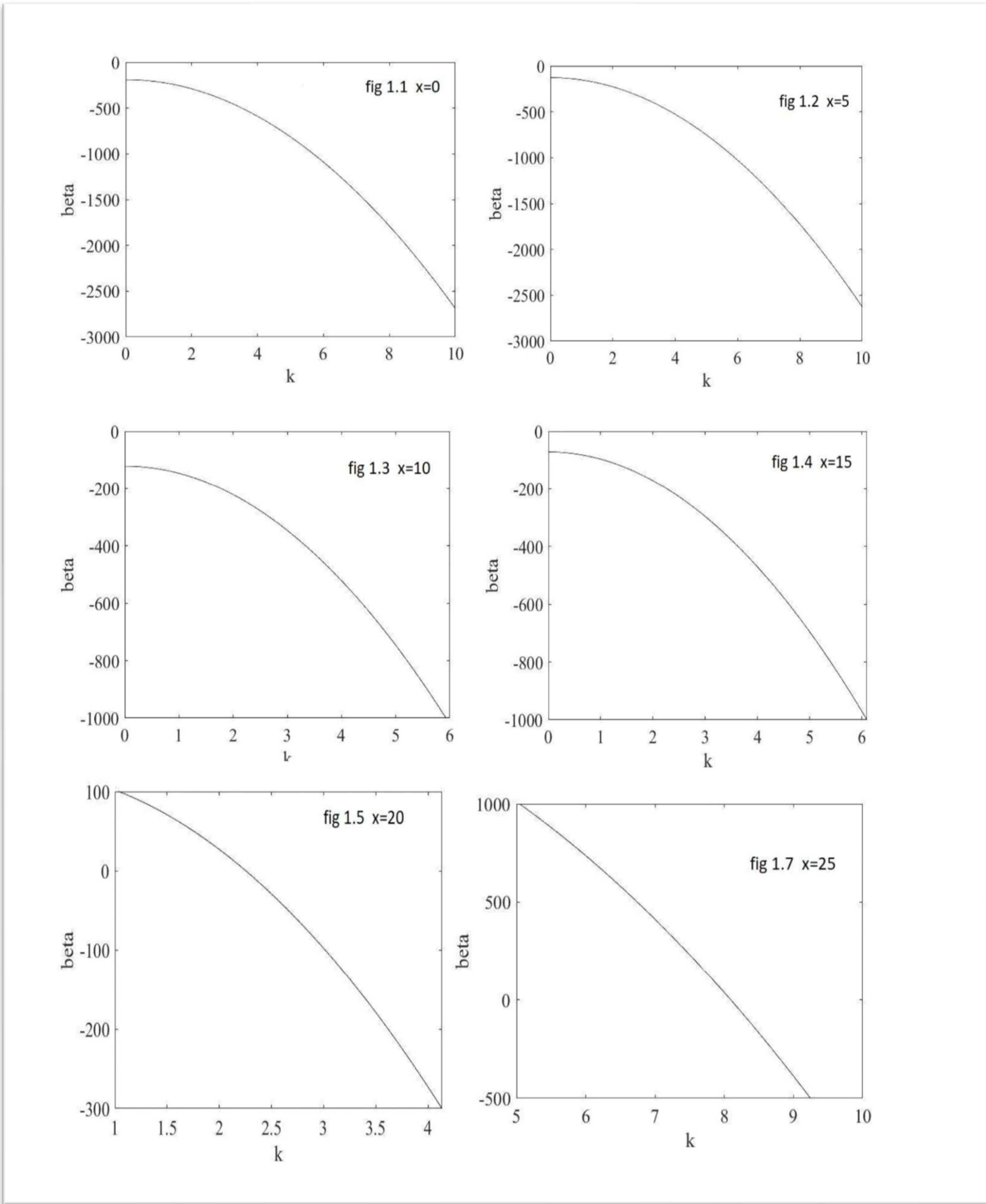
3. In fig- 3, y0= [0.01,0.0007,0.01, -0.02] and amplitude of oscillation first decreases till x=30(approximately) after that it increases continuously.

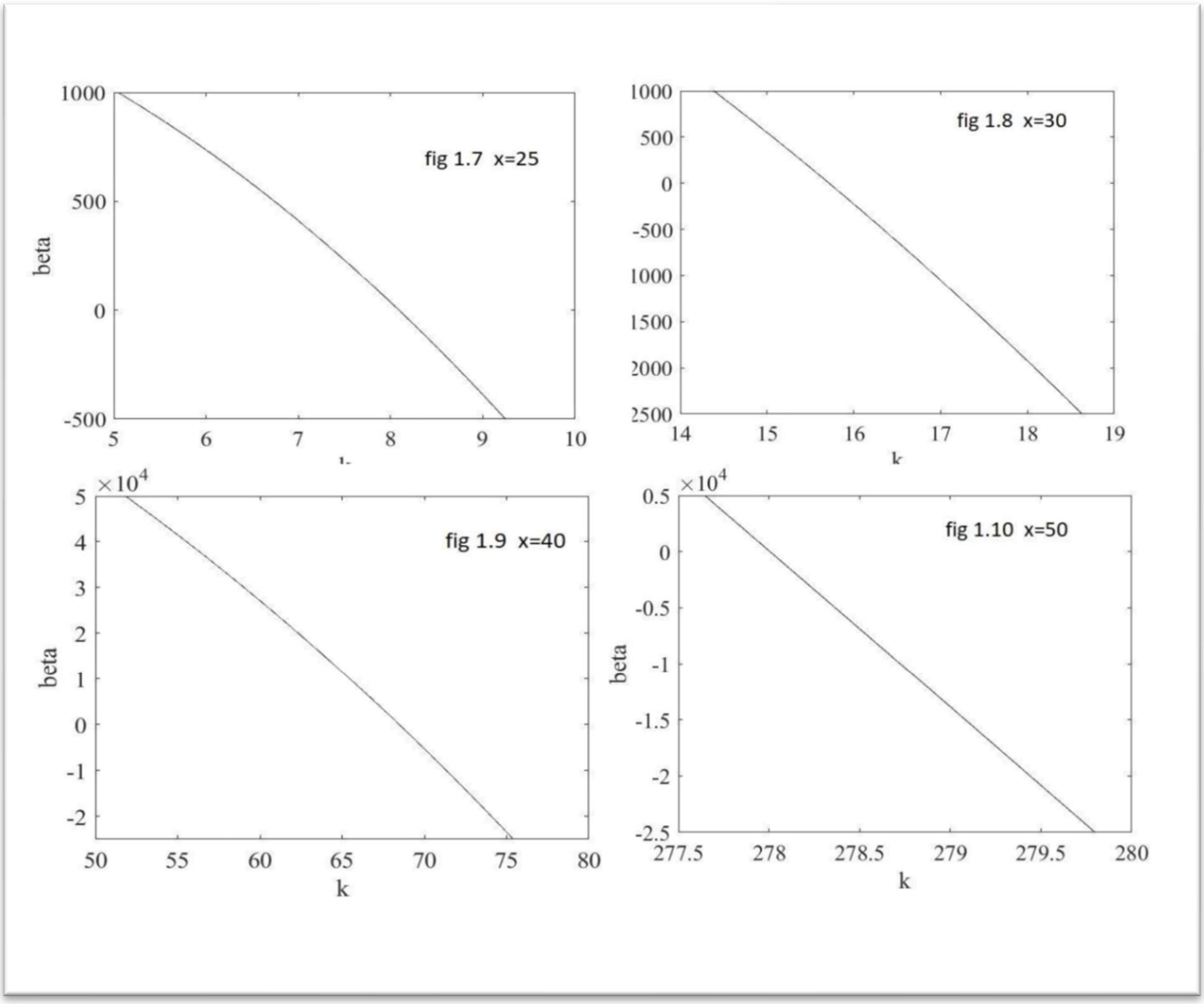
4. In fig-4, y0= [0.01,0.257,0.01, -0.5] ,amplitude decreases till x=20 after this it becomes almost constant.

5. In fig -5 y0= [0.1,0.1,0.1, -0.0005] ,initially the amplitude of oscillation is higher and it decreases to very small value after x=10.

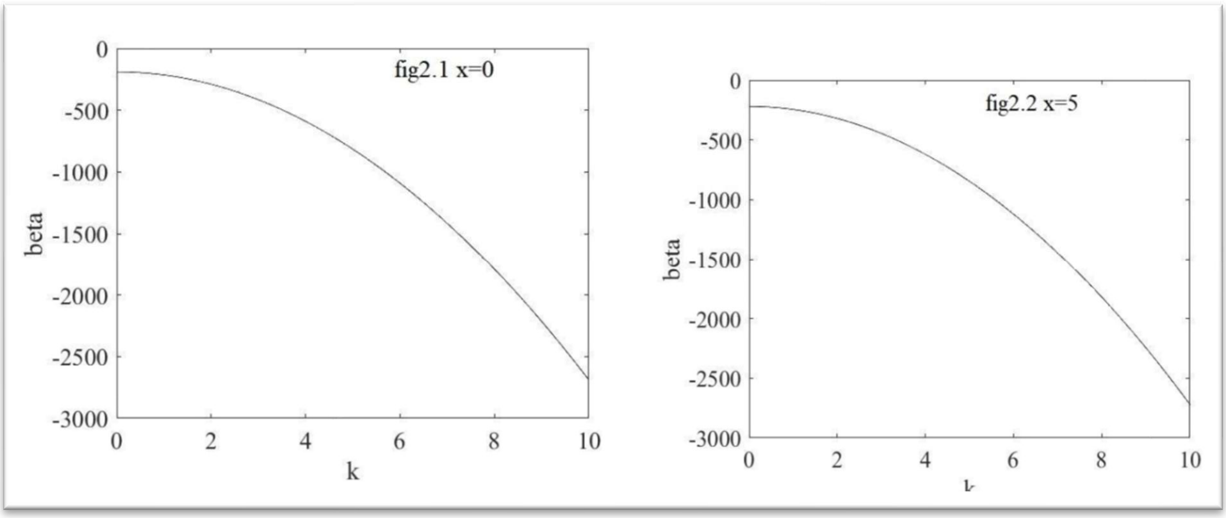
Result -2.Growth rate (β) Vs. wavenumber (κ)-

β vs. κ for steady-state, fig-1





<u>β vs. κ for steady-state ,fig-2</u>



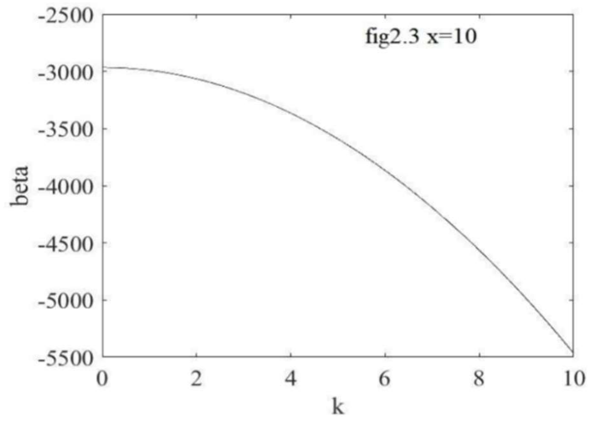


fig2.3 x=10
beta
k
-2500
-3000
-3500
-4000
-4500
-5000
-5500
0
2
4
6
8
10

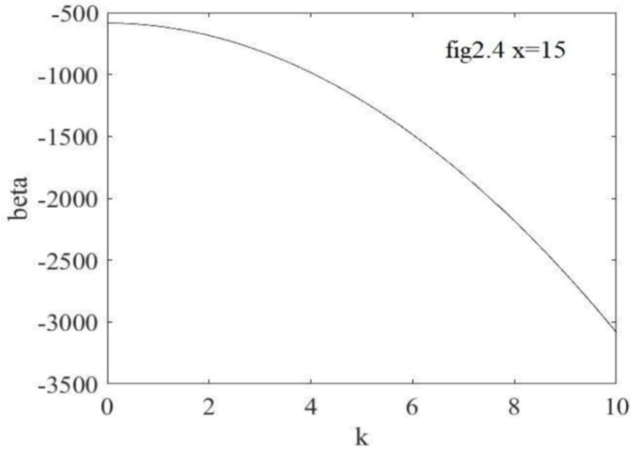


fig2.4 x=15
beta
k
-500
-1000
-1500
-2000
-2500
-3000
-3500
0
2
4
6
8
10

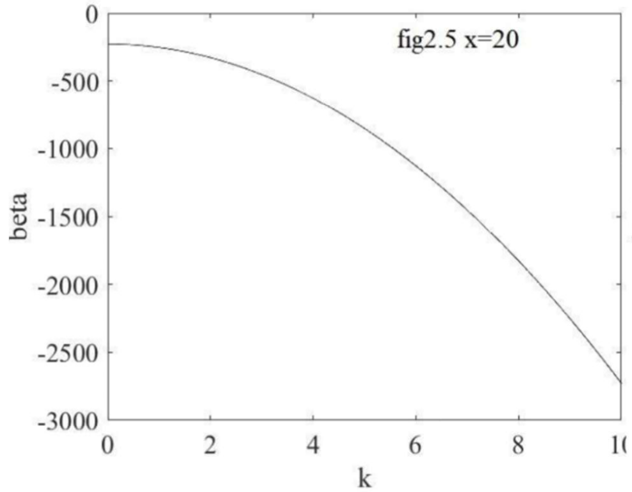


fig2.5 x=20
beta
k
0
-500
-1000
-1500
-2000
-2500
-3000
0
2
4
6
8

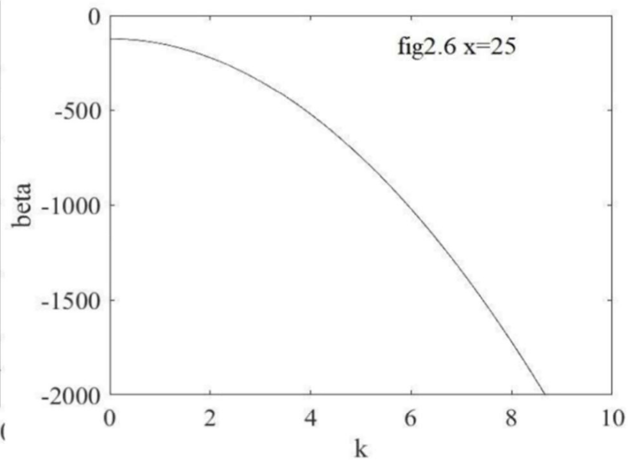


fig2.6 x=25
beta
k
0
-500
-1000
-1500
-2000
0
2
4
6
8
10

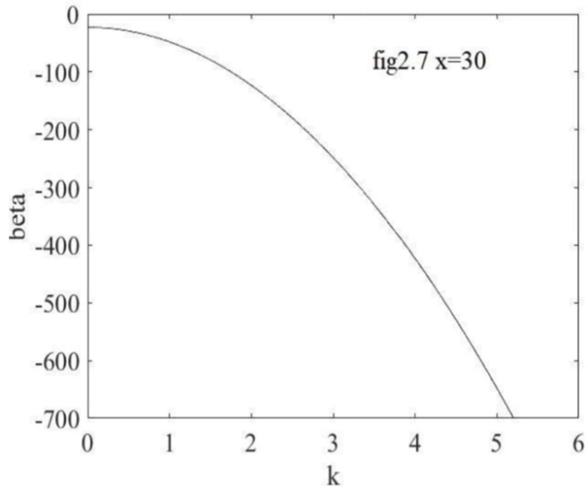


fig2.7 x=30
beta
k
0
-100
-200
-300
-400
-500
-600
-700
0
1
2
3
4
5
6

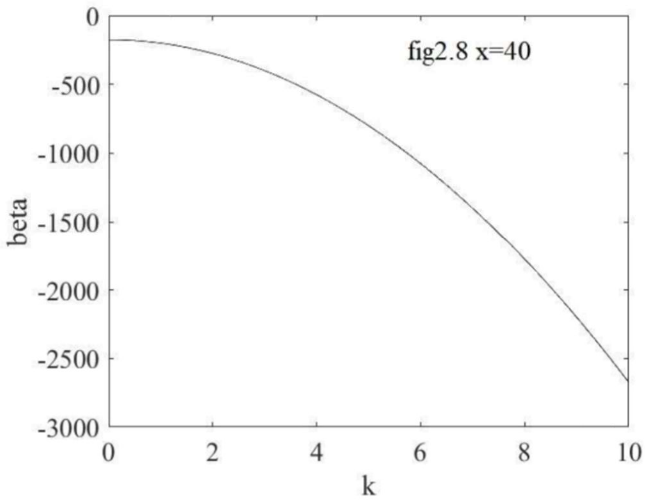
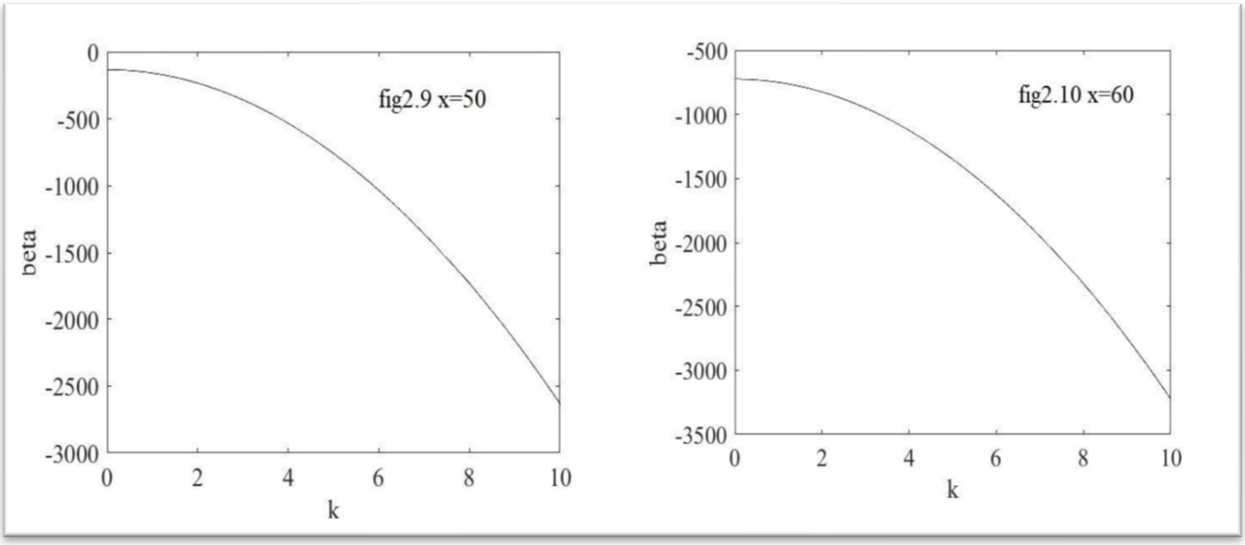
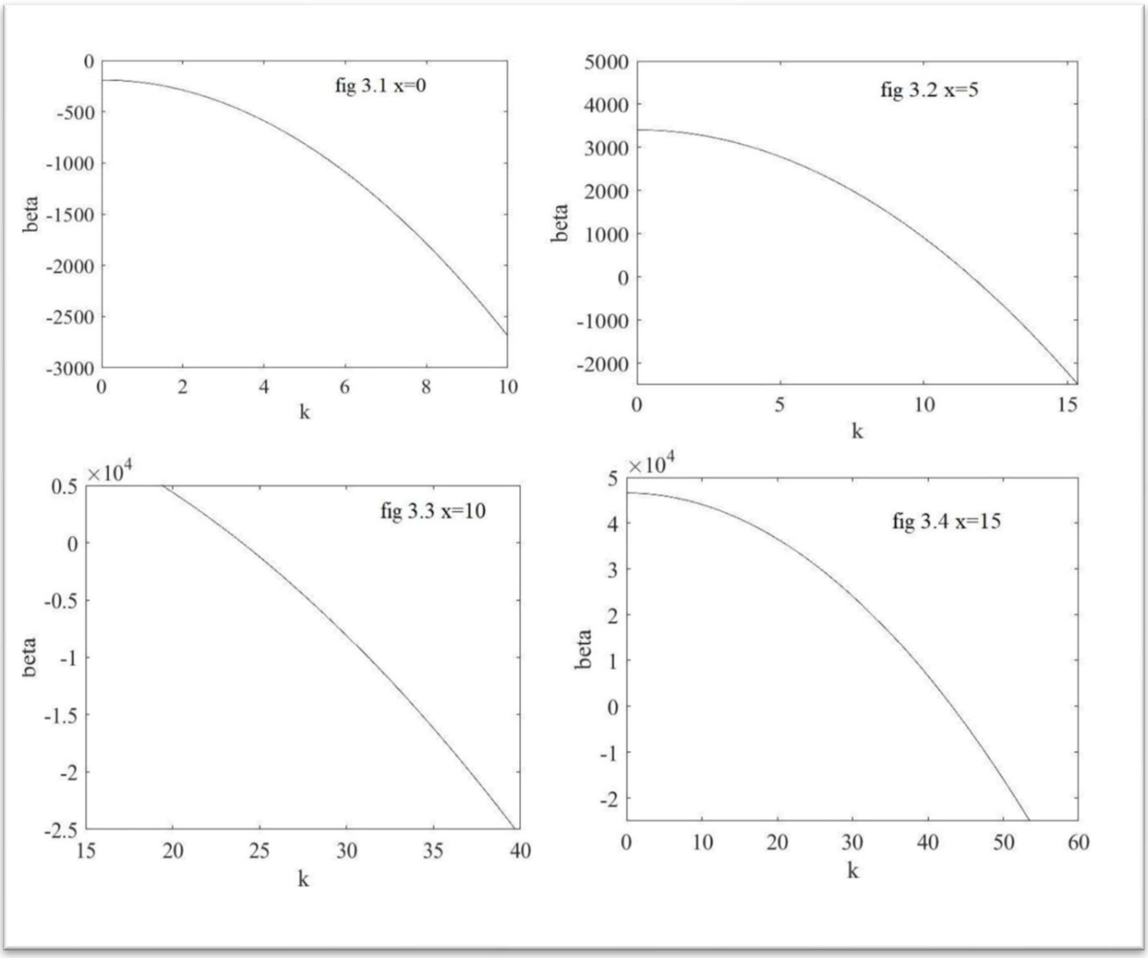


fig2.8 x=40
beta
k
0
-500
-1000
-1500
-2000
-2500
-3000
0
2
4
6
8
10



β vs. κ for steady-state ,fig-3



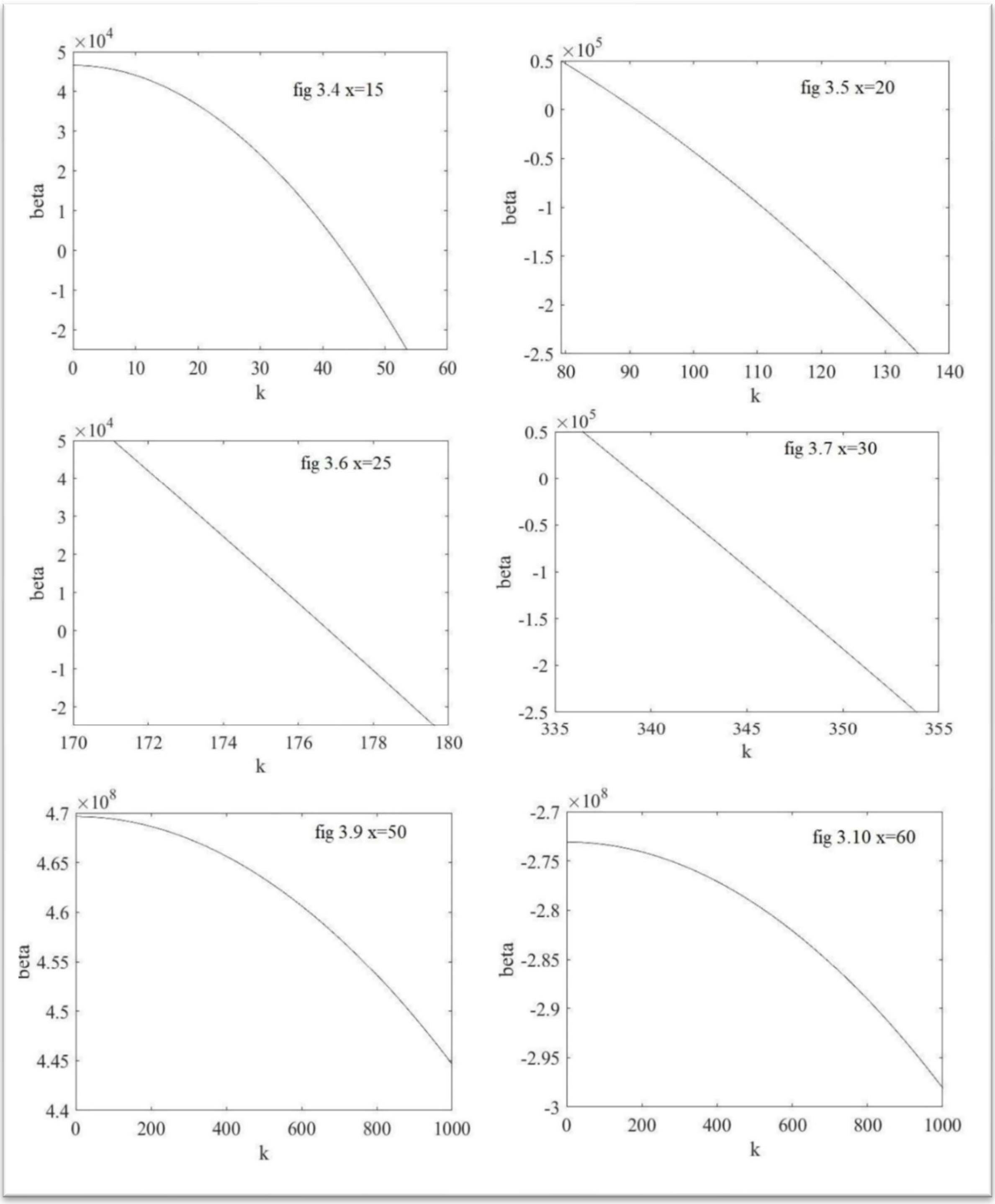
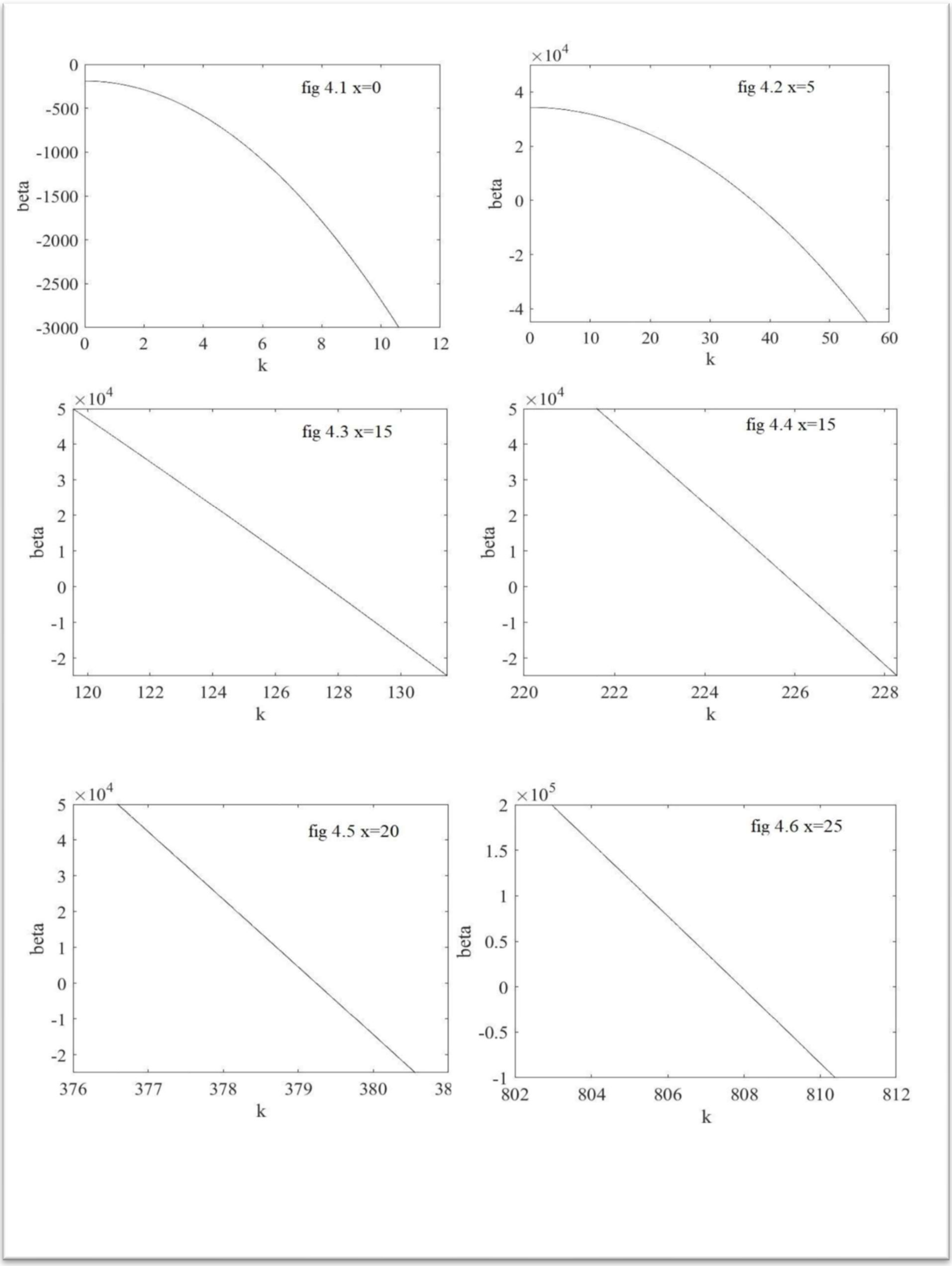
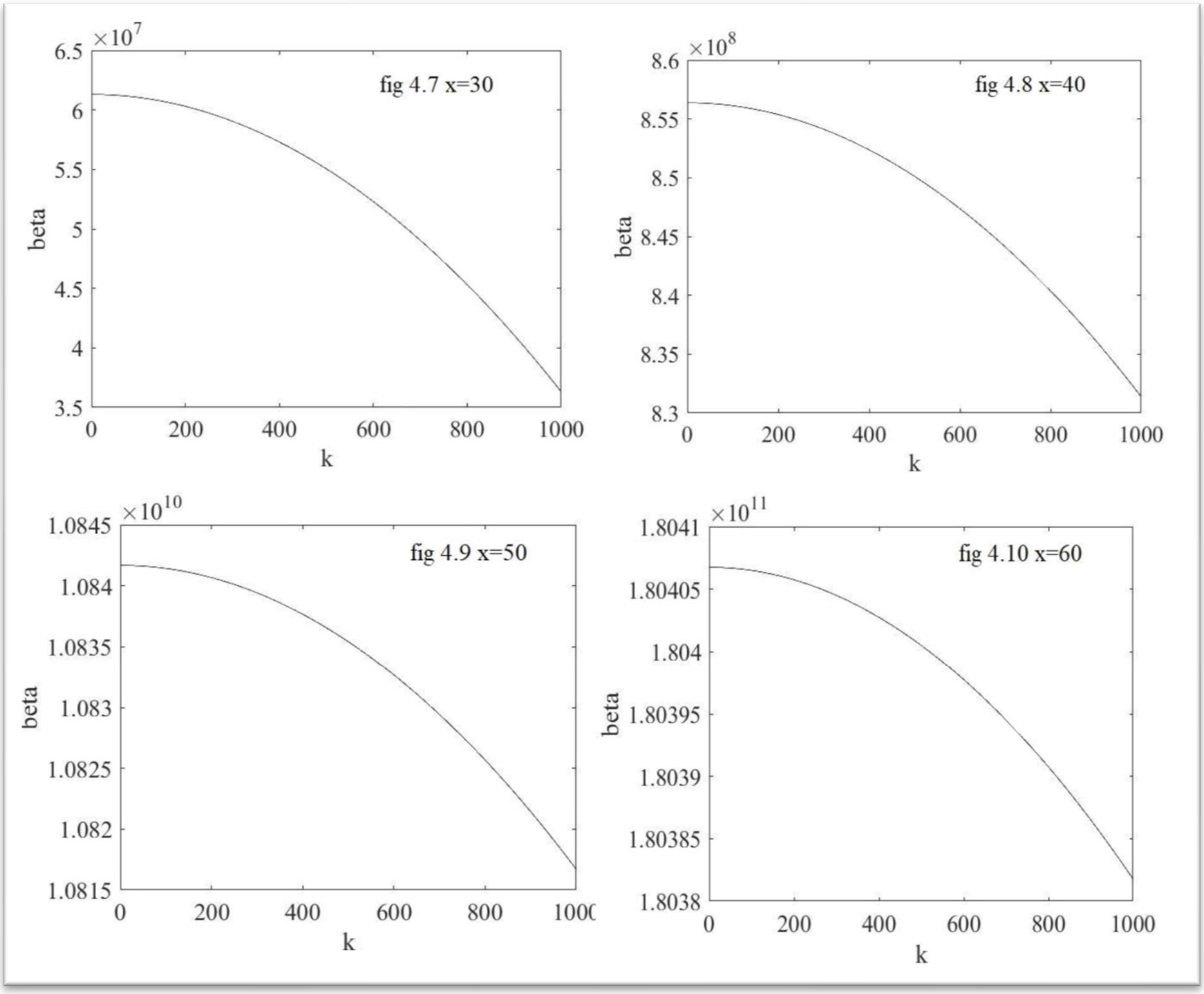


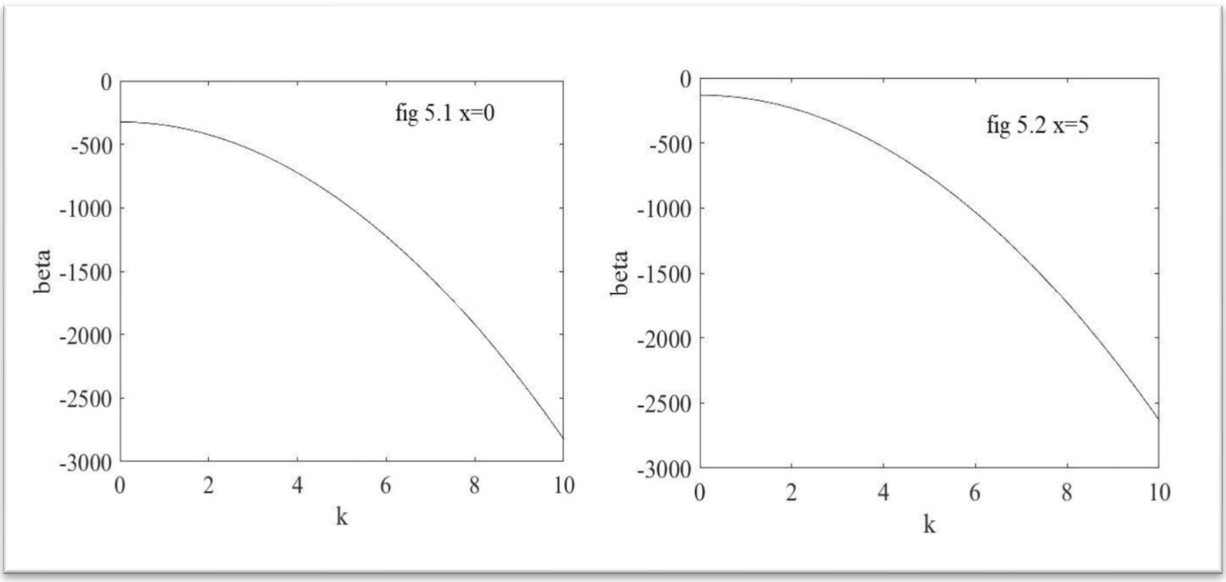
fig 3.4 x=15
fig 3.5 x=20
fig 3.6 x=25
fig 3.7 x=30
fig 3.9 x=50
fig 3.10 x=60
beta
k

β vs. κ for steady-state,fig-4





β vs. κ for steady-state,fig-5



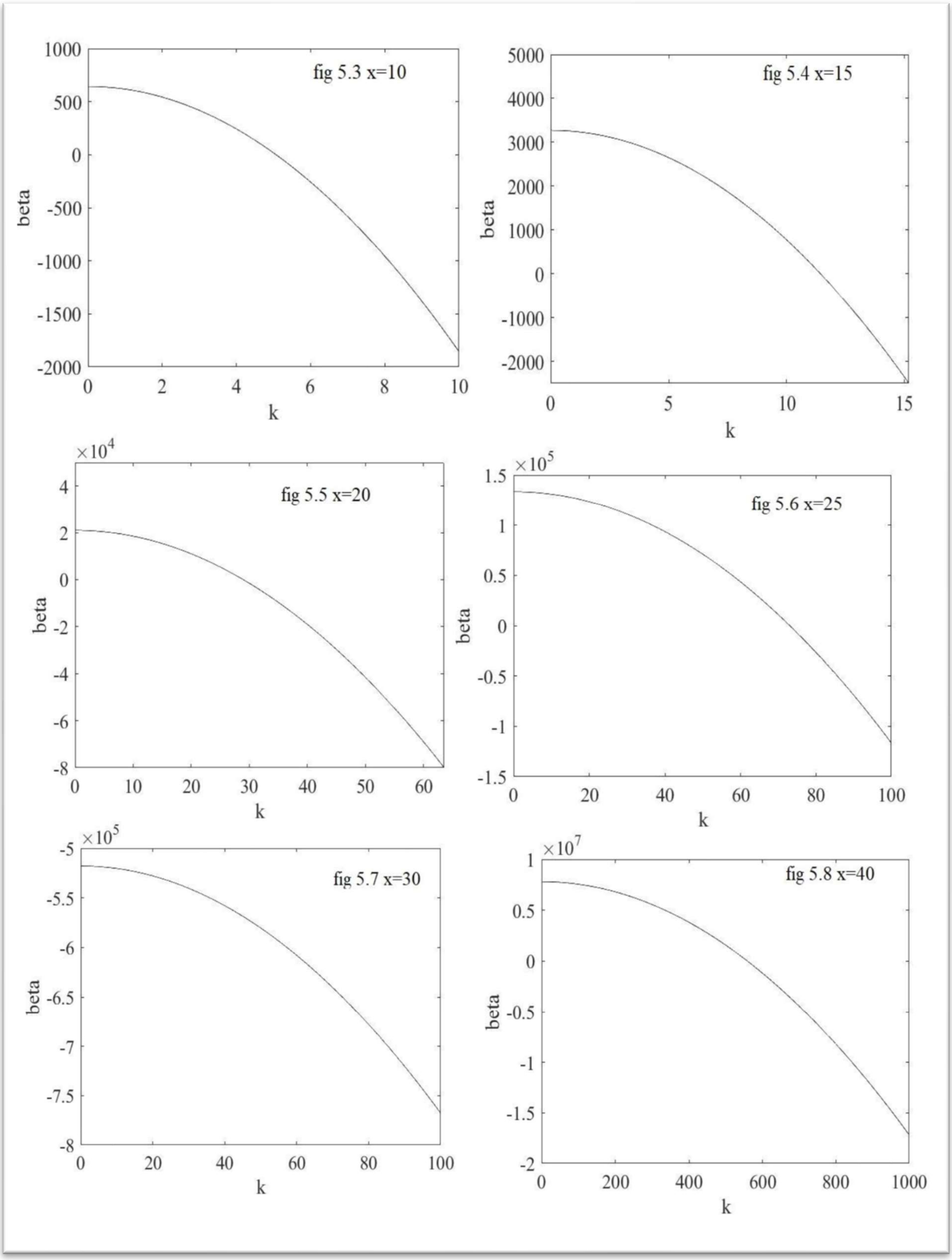


fig 5.3 x=10
1000
500
0
-500
-1000
-1500
-2000
0
2
4
6
8
10
beta
k
fig 5.4 x=15
5000
4000
3000
2000
1000
0
-1000
-2000
0
5
10
15
beta
k
$\times 10^4$
fig 5.5 x=20
4
2
0
-2
-4
-6
-8
0
10
20
30
40
50
60
beta
k
$\times 10^5$
fig 5.6 x=25
1.5
1
0.5
0
-0.5
-1
-1.5
0
20
40
60
80
100
beta
k
$\times 10^5$
fig 5.7 x=30
-5
-5.5
-6
-6.5
-7
-7.5
-8
0
20
40
60
80
100
beta
k
$\times 10^7$
fig 5.8 x=40
1
0.5
0
-0.5
-1
-1.5
-2
0
200
400
600
800
1000
beta
k

For all the steady states plotted above, fig 1-5, the stability of the system for different wavenumber at different positions is studied by plotting the graphs between β and κ using equation 9.

<u>For Steady state solution with y0= [0.01,0.007,0.01, -0.000110],fig- 1</u>
At x=0 fig1.1, β is negative for all k.
At x=5 fig1.2, β is negative for all k.
At x=10 fig1.3, β is negative for all k.
At x=15 fig1.4, β is negative for all k.
At x=20 fig1.5, β is negative for k >2.25.
At x=23 fig1.6, β is negative for k>4.5.
At x=25 fig1.7, β is negative for k >8.
At x=30 fig1.8, β is negative for k>15.8.
At x=40 fig1.9, β is negative for k>67.
At x=50 fig1.10, β is negative for k>278.

Initially, the system is stable for all wavenumbers. As x increases, the wavenumber after which the system becomes stable also increases.

<u>For steady-state ,fig- 2</u>
Beta is negative for all k at all x.Therefore the system is stable for all x in the domain. (0-60)

<u>For steady-state ,fig- 3</u>
At x=0 fig3.1, beta is negative for all k.
At x=5 fig3.2, beta is negative for k>12.
At x=10 fig3.3, beta is negative for k>25.
At x=15 fig3.4, beta is negative for k>45.
At x=20 fig3.5, beta is negative for k>92.
At x=25 fig3.6, beta is negative for k>178.
At x=30 fig3.7, beta is negative for k>341.
At x=40 fig3.8, beta is positive for all k up to 1000.
At x=50 fig3.9, beta is positive for all k up to 1000.
At x=60 fig 3.10, beta is negative for all k.

Initially, the system was stable, as x increases, the wave number at which the system is stable also increases continuously.

For steady-state, fig- 4

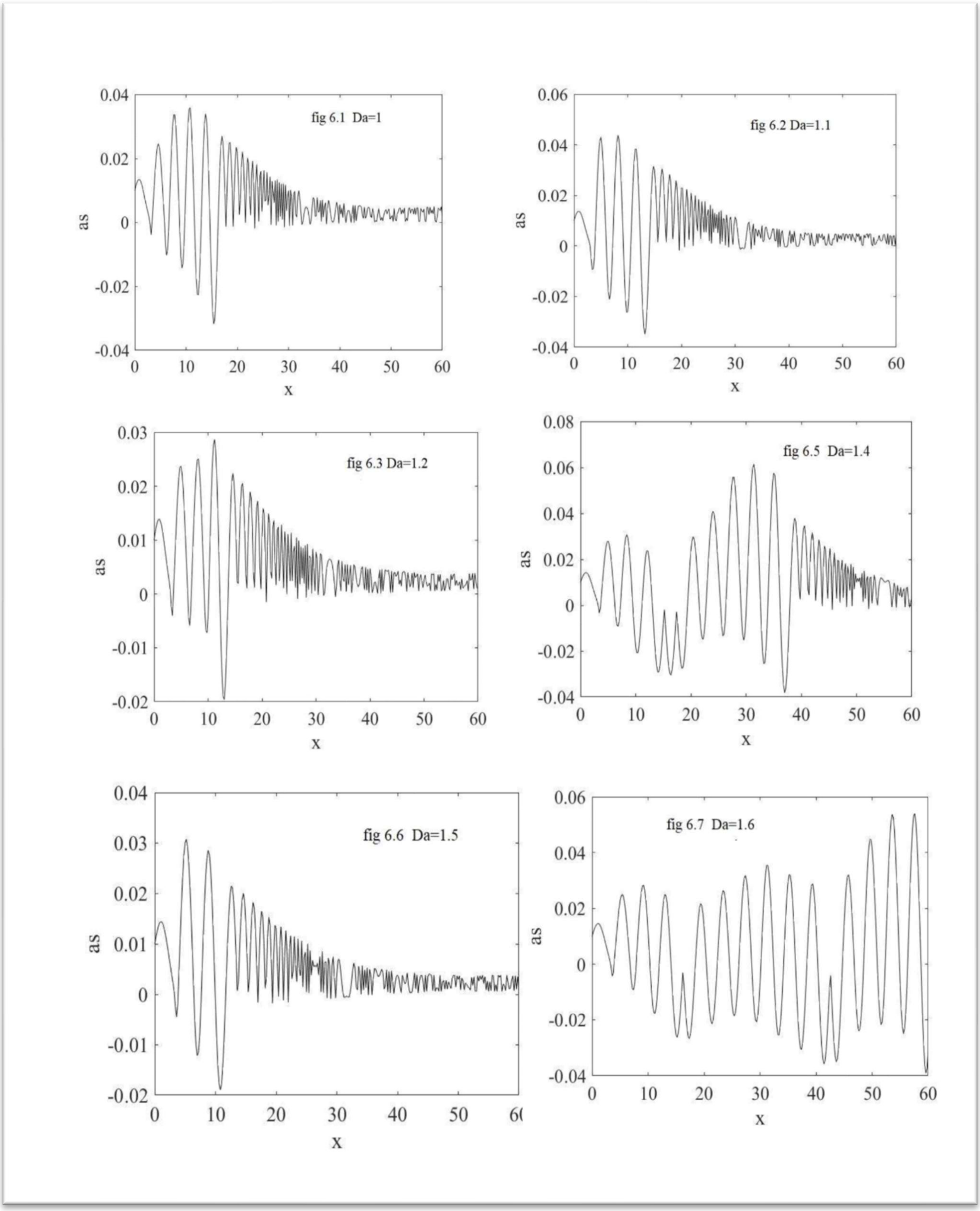
At x=0 fig4.1, beta is negative for all k.
At x=5 fig4.2, beta is negative for k>38.
At x=10 fig4.3, beta is negative for k>128.
At x=15 fig4.4, beta is negative for k>226.
At x=20 fig4.5, beta is negative for k>379.
At x=25 fig4.6, beta is negative for k>808.
At x=30 fig4.7, beta is positive for all k up to 1000.
At x=40 fig4.8, beta is positive for all k up to 1000.
At x=50 fig4.9, beta is positive for all k up to 1000.
At x=60 fig4.10, beta is positive for all k up to 1000.

Initially, the system was stable, as x increases, the wave number at which the system is stable also increases continuously.

For steady-state, fig- 5

At x=0 fig5.1, beta is negative for all k.
At x=5 fig5.2, beta is negative for all k.
At x=10 fig5.3, beta is negative for k>5.
At x=15 fig5.4, beta is negative for k>12.
At x=20 fig5.5, beta is negative for k>30.
At x=25 fig5.6, beta is negative for k>75.
At x=30 fig 5.7, beta is negative for all k.
At x=40 fig 5.8,beta is negative for k>550.
At x=50,60 beta is positive for all k up to 1000.
Initially the system is stable for all k, but as the x increases, the value of wavenumber also increases. At x=30 system is stable for all values of κ.

Result -3.Variation of steady-state with D_a



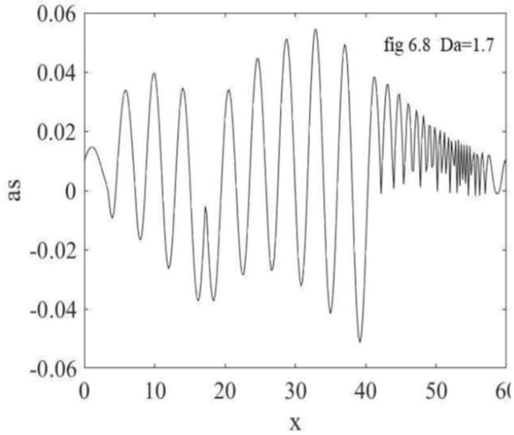


fig 6.8 Da=1.7
as
x

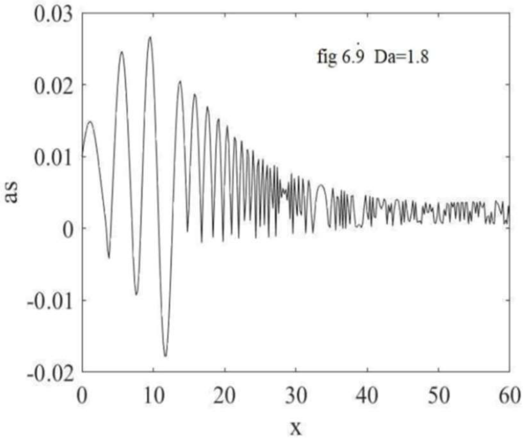


fig 6.9 Da=1.8
as
x

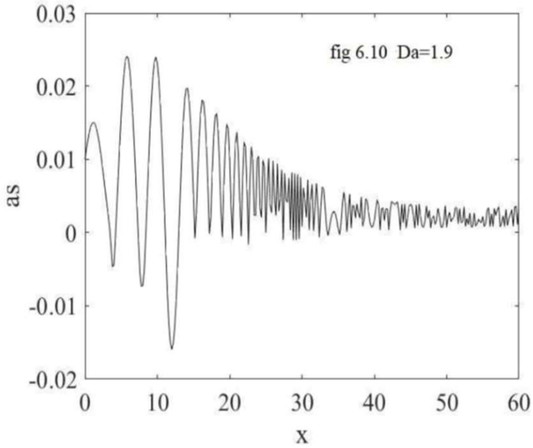


fig 6.10 Da=1.9
as
x

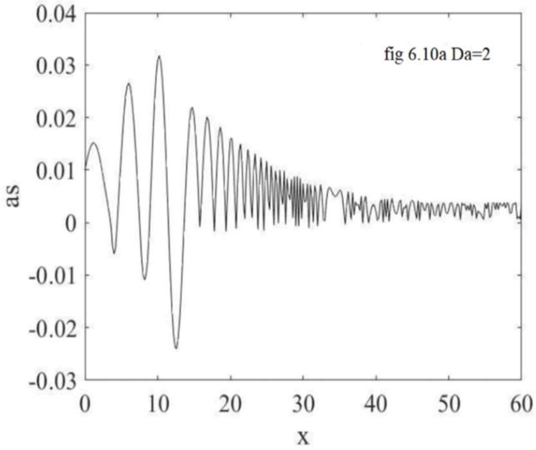


fig 6.10a Da=2
as
x

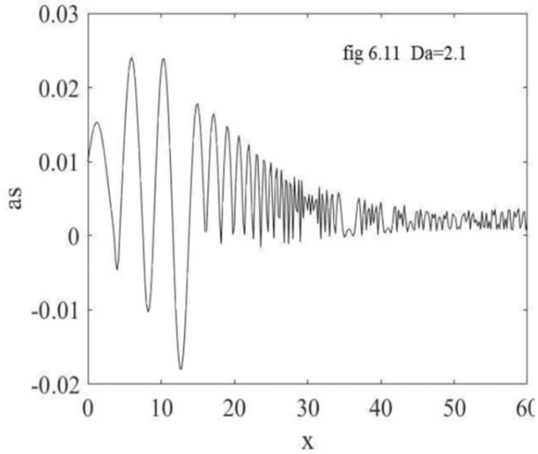


fig 6.11 Da=2.1
as
x

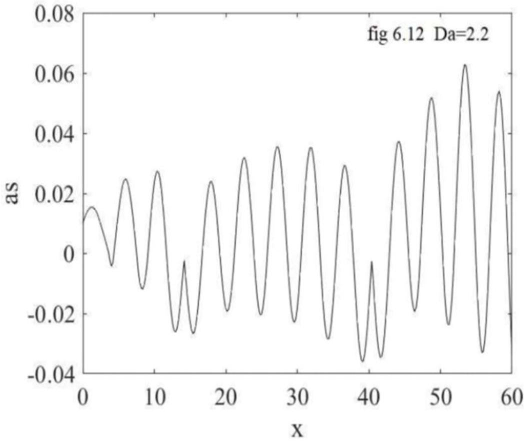


fig 6.12 Da=2.2
as
x

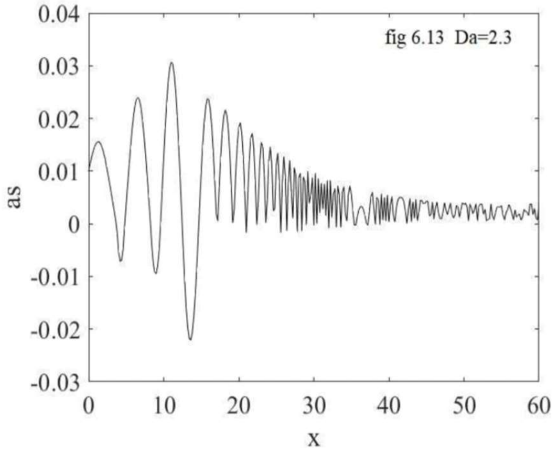


fig 6.13 Da=2.3
as
x

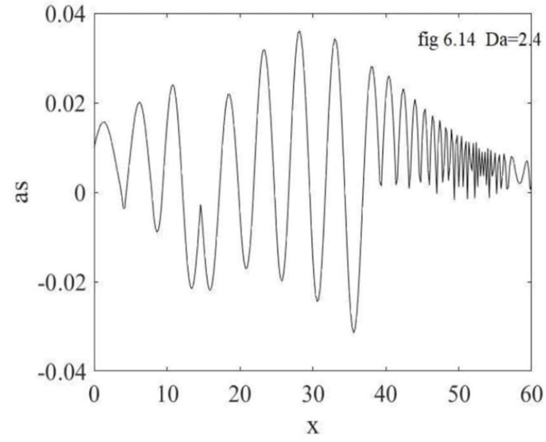


fig 6.14 Da=2.4
as
x

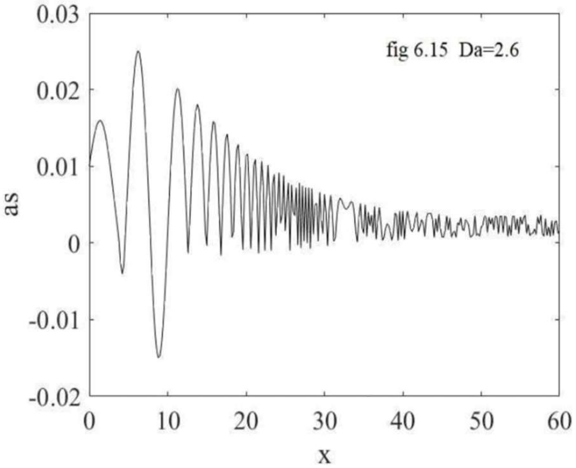


fig 6.15 Da=2.6
as
x

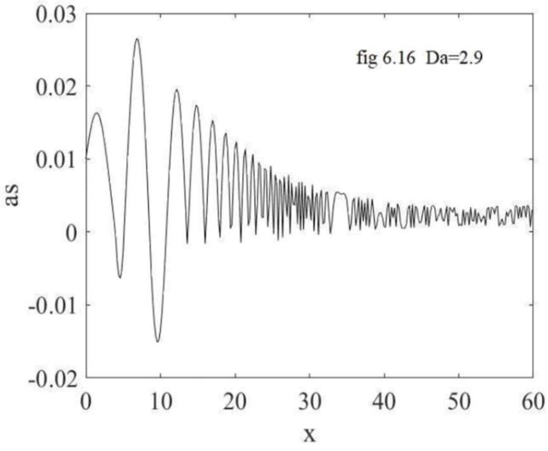


fig 6.16 Da=2.9
as
x

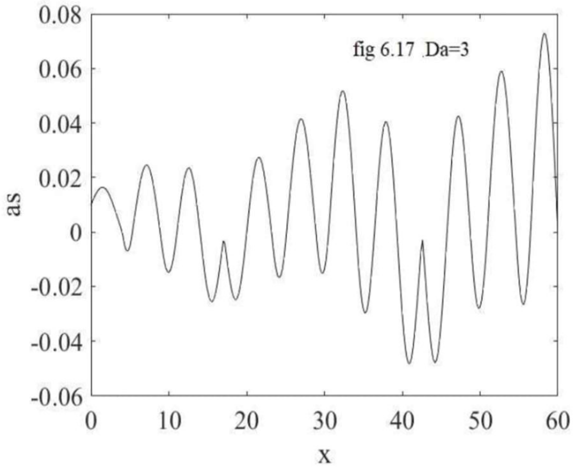


fig 6.17 Da=3
as
x

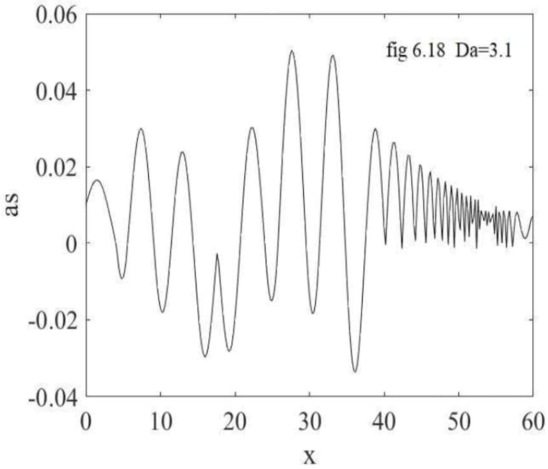


fig 6.18 Da=3.1
as
x

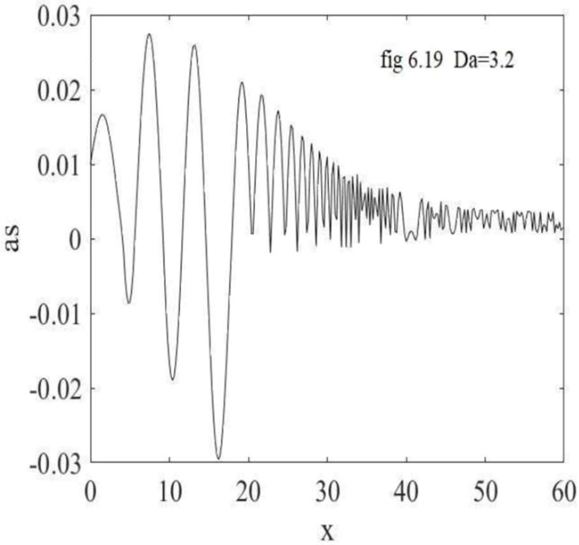


fig 6.19 Da=3.2

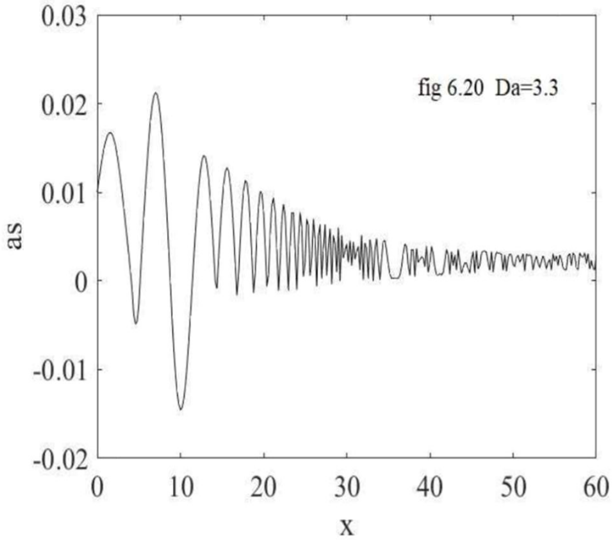


fig 6.20 Da=3.3

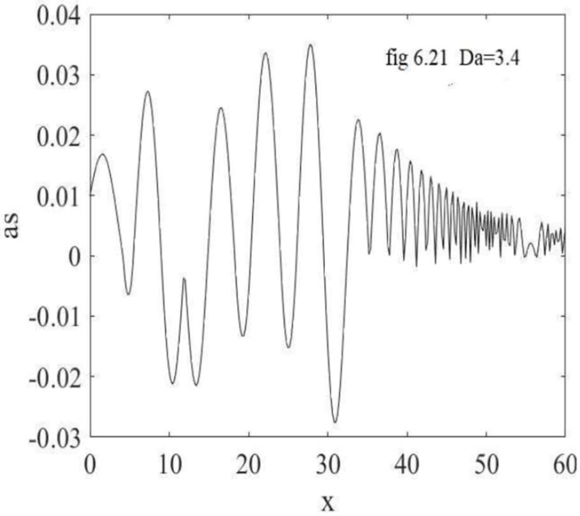


fig 6.21 Da=3.4

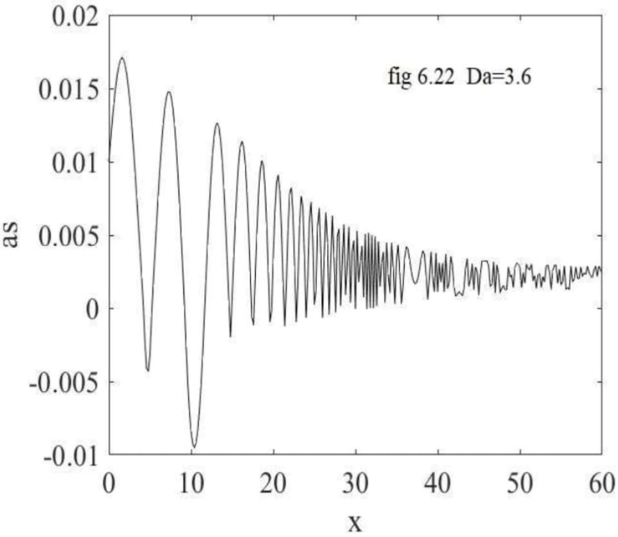


fig 6.22 Da=3.6

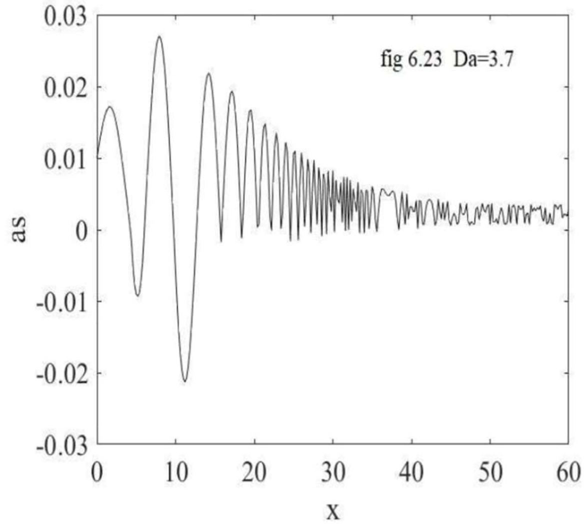


fig 6.23 Da=3.7

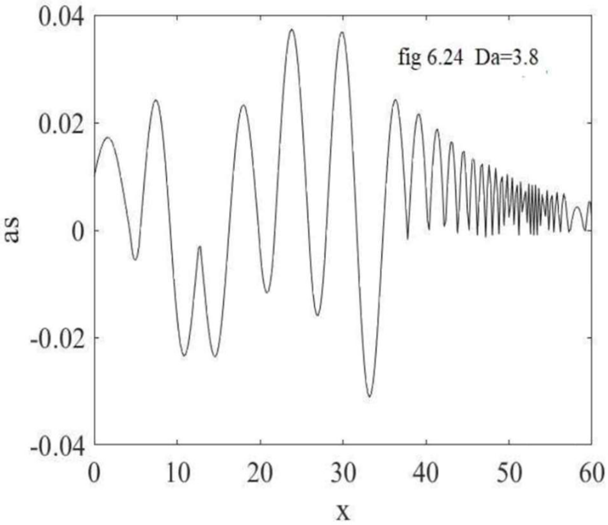


fig 6.24 Da=3.8

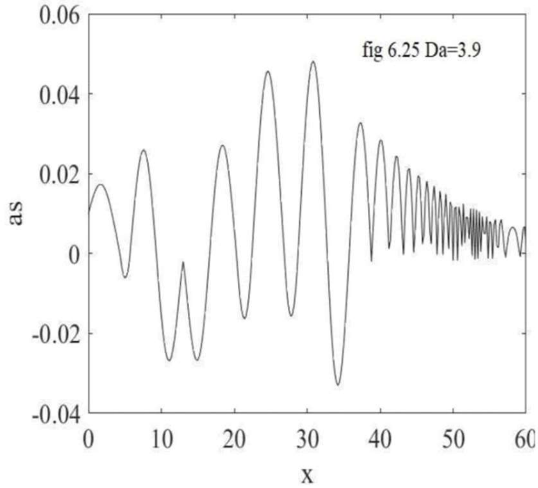


fig 6.25 Da=3.9
as
x

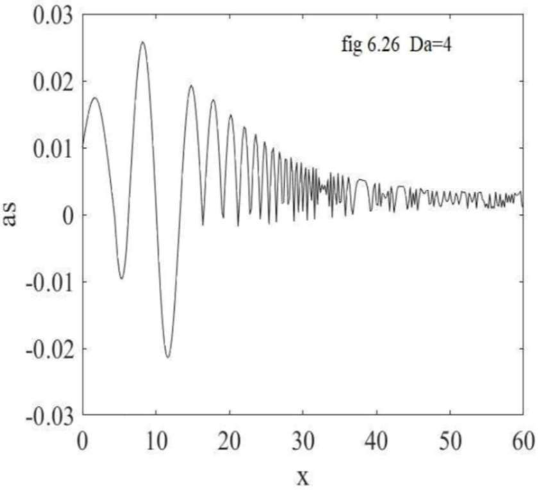


fig 6.26 Da=4
as
x

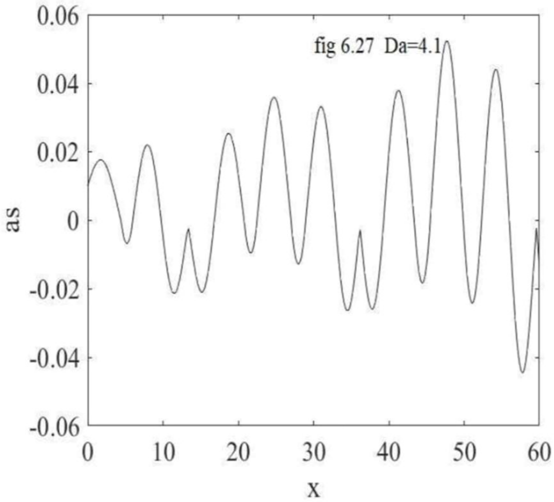


fig 6.27 Da=4.1
as
x

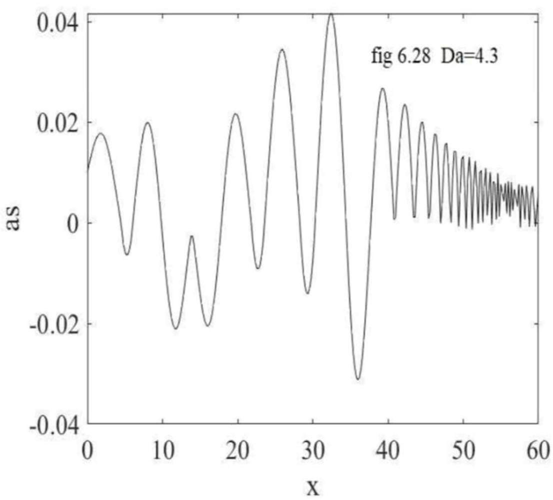


fig 6.28 Da=4.3
as
x

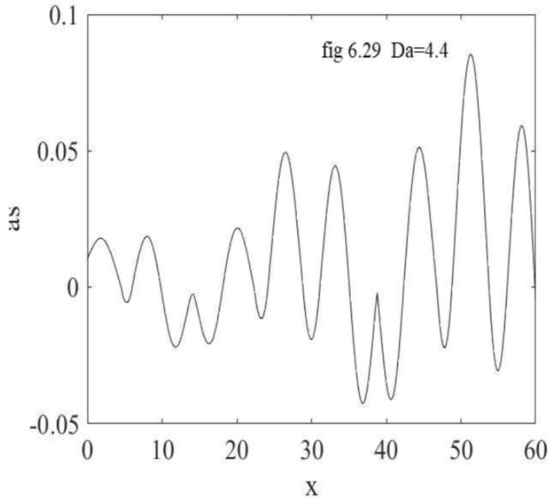


fig 6.29 Da=4.4
as
x

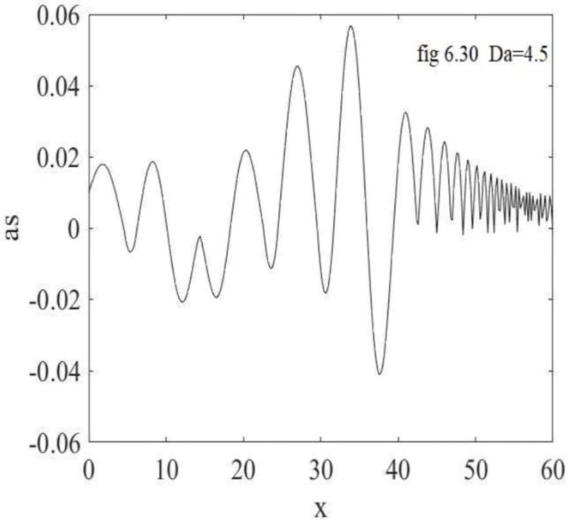


fig 6.30 Da=4.5
as
x

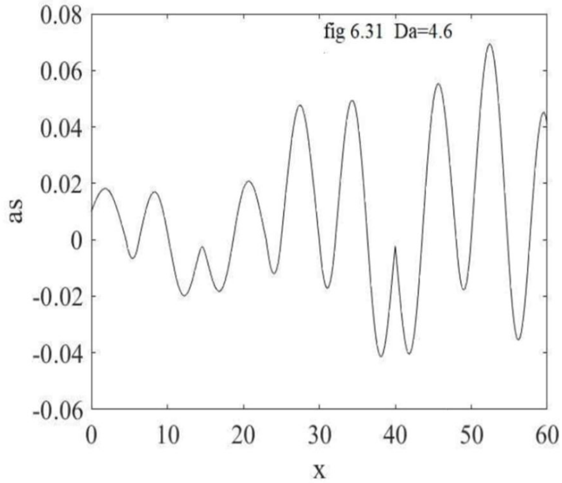


fig 6.31 Da=4.6
as
x
0.08
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
0
10
20
30
40
50
60

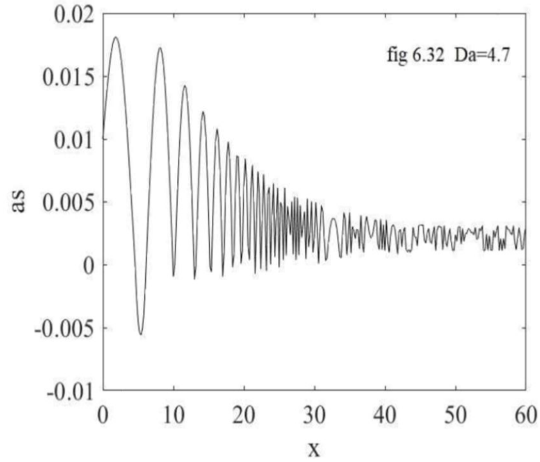


fig 6.32 Da=4.7
as
x
0.02
0.015
0.01
0.005
0
-0.005
-0.01
0
10
20
30
40
50
60

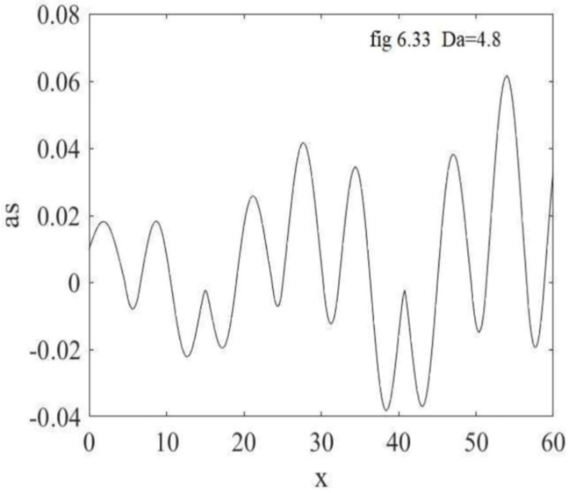


fig 6.33 Da=4.8
as
x
0.08
0.06
0.04
0.02
0
-0.02
-0.04
0
10
20
30
40
50
60

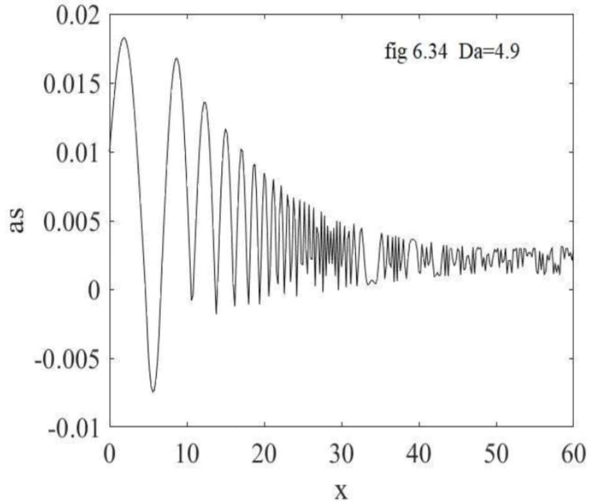


fig 6.34 Da=4.9
as
x
0.02
0.015
0.01
0.005
0
-0.005
-0.01
0
10
20
30
40
50
60

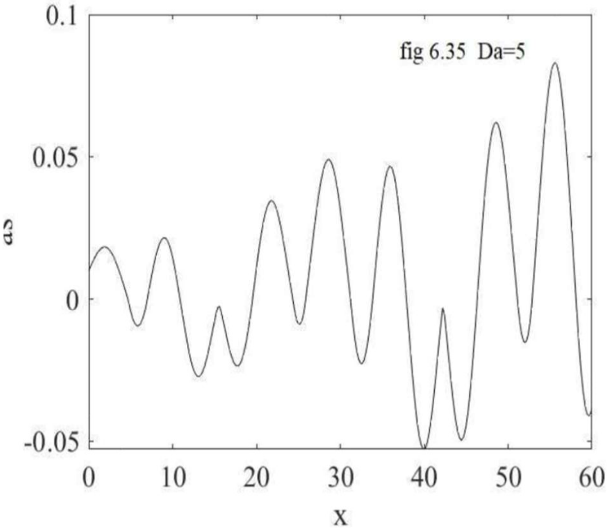


fig 6.35 Da=5
x
0.1
0.05
0
-0.05
0
10
20
30
40
50
60

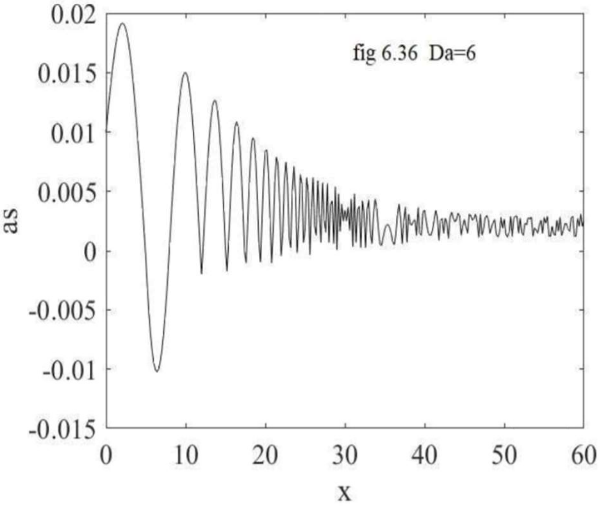


fig 6.36 Da=6
as
x
0.02
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
0
10
20
30
40
50
60

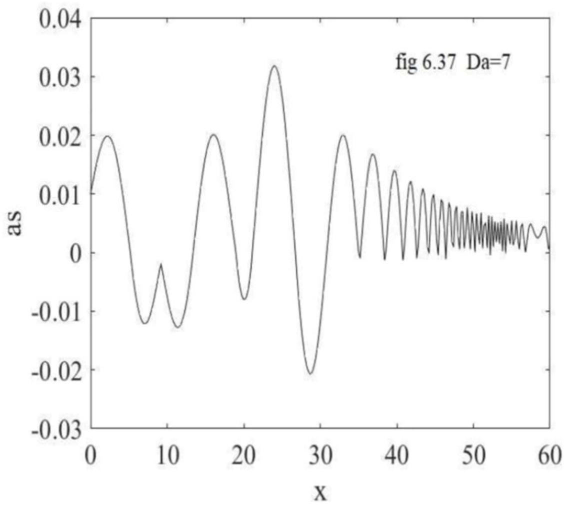


fig 6.37 Da=7
as
x

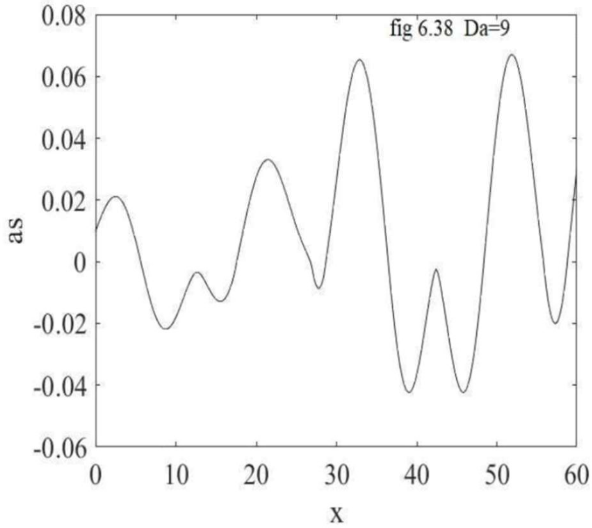


fig 6.38 Da=9
as
x

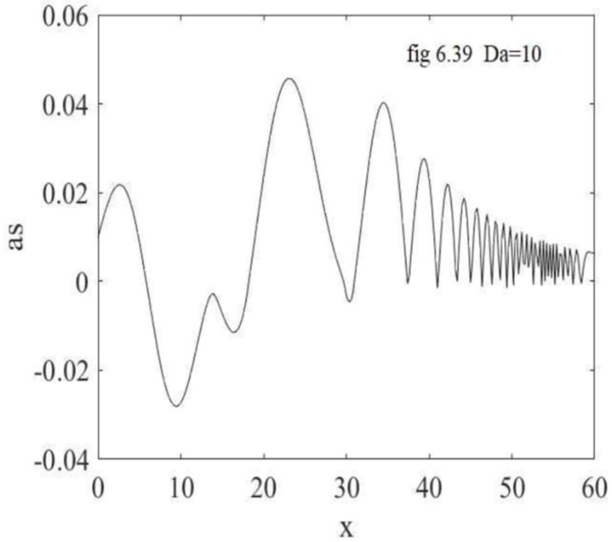


fig 6.39 Da=10
as
x

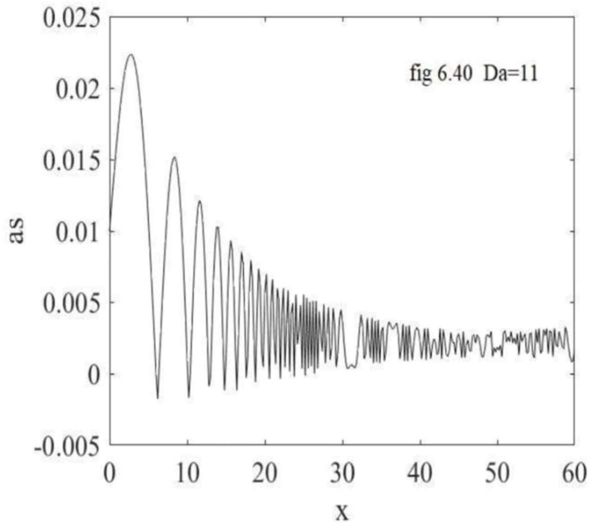


fig 6.40 Da=11
as
x

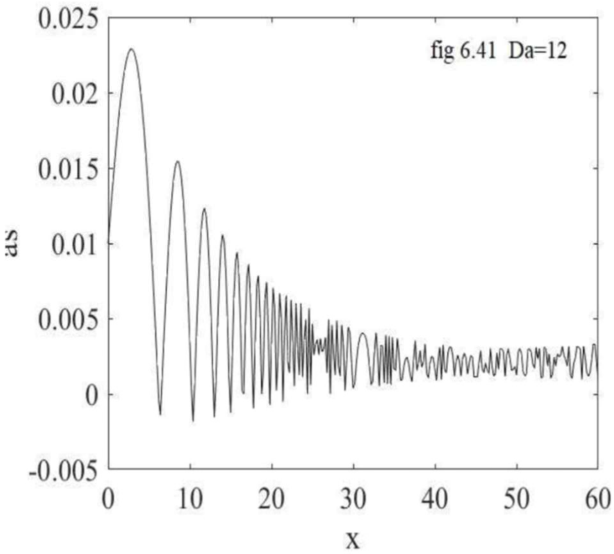


fig 6.41 Da=12
as
x

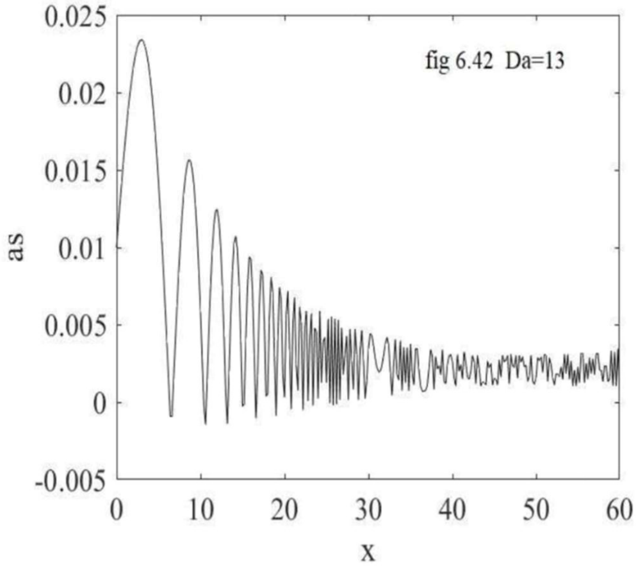


fig 6.42 Da=13
as
x

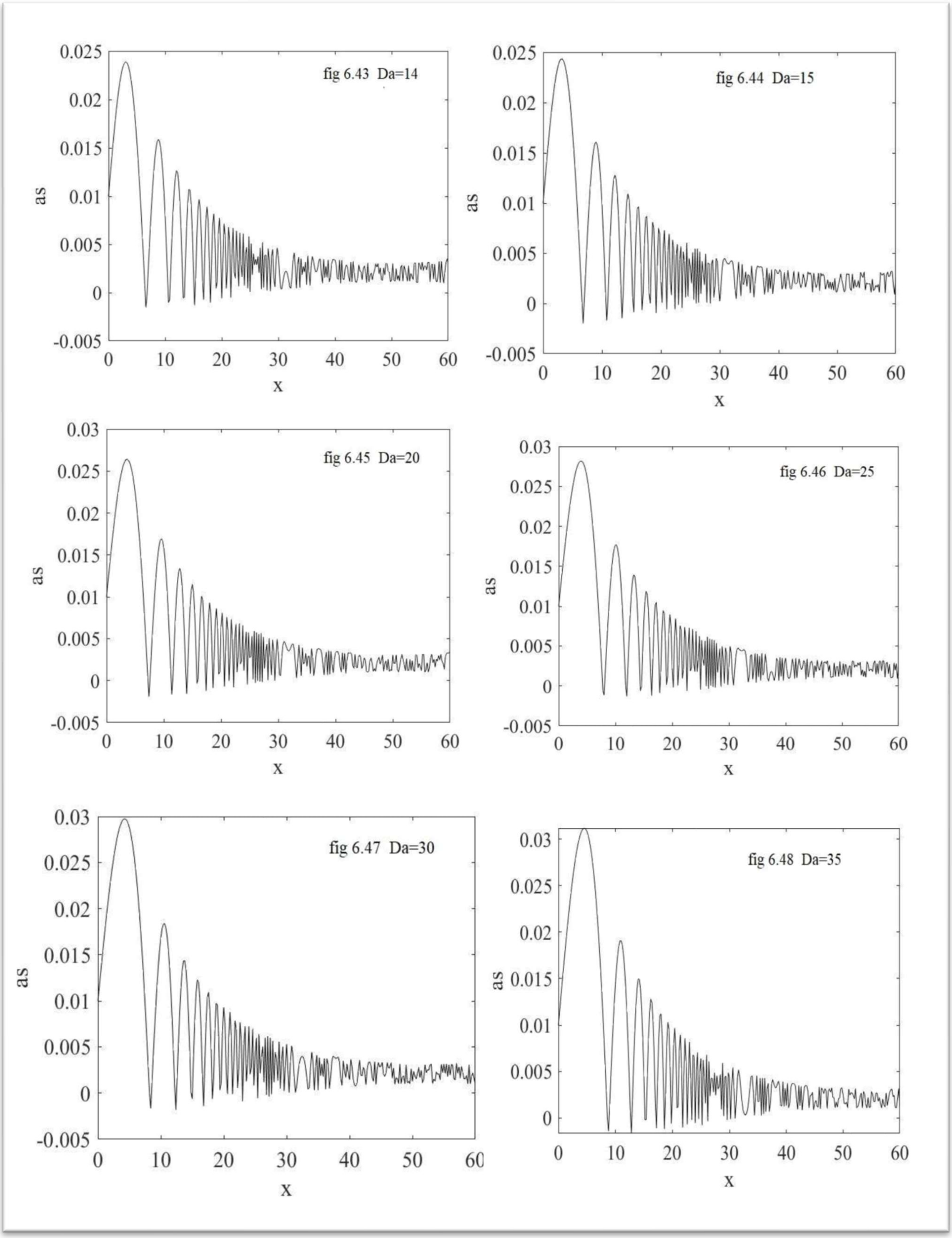


fig 6.43 Da=14
fig 6.44 Da=15
fig 6.45 Da=20
fig 6.46 Da=25
fig 6.47 Da=30
fig 6.48 Da=35
as
x

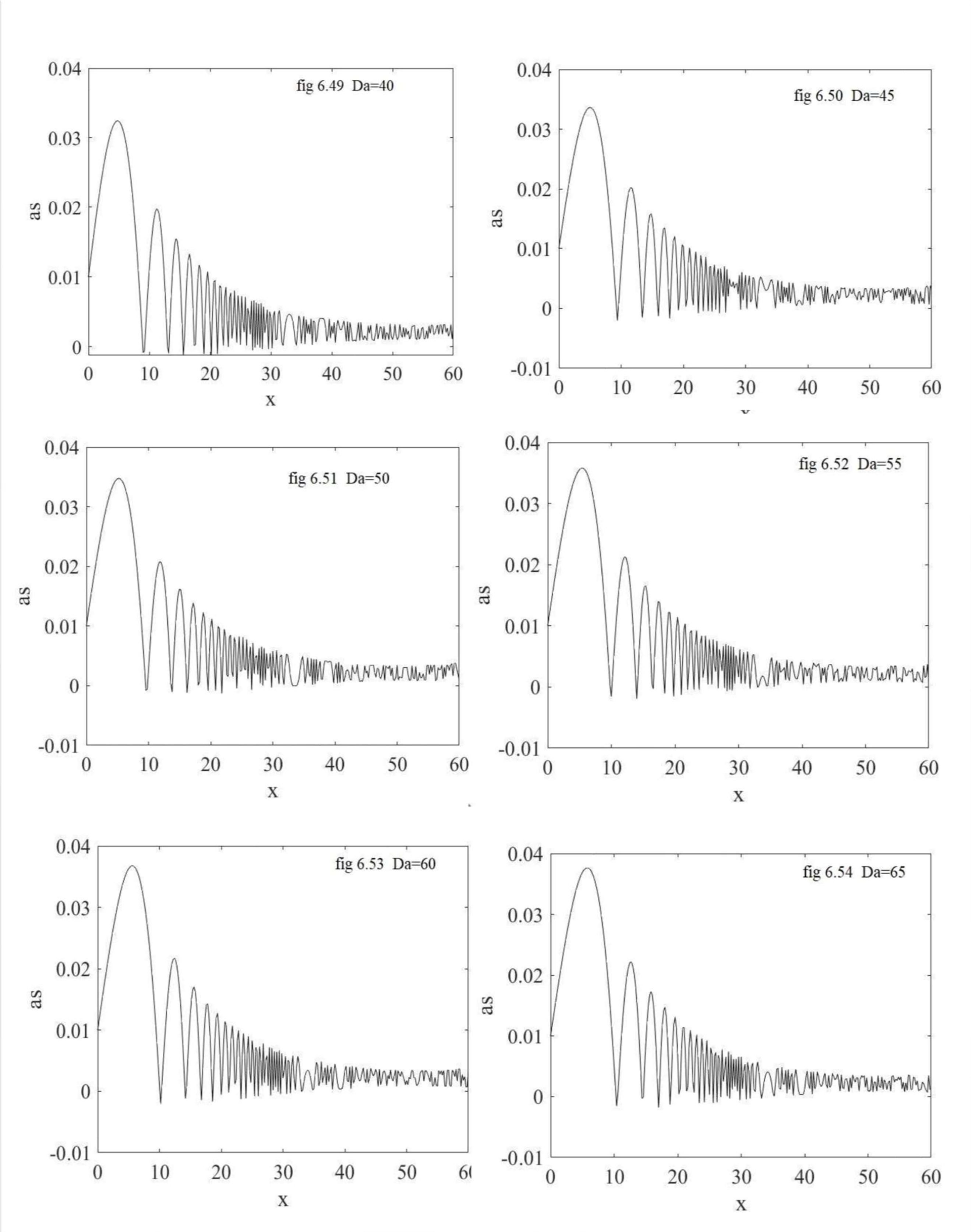


fig 6.49 Da=40
fig 6.50 Da=45
fig 6.51 Da=50
fig 6.52 Da=55
fig 6.53 Da=60
fig 6.54 Da=65
as
x

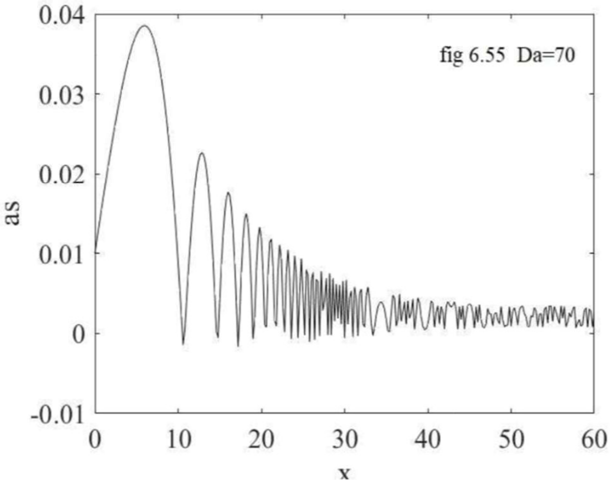


fig 6.55 Da=70
as
x
0.04
0.03
0.02
0.01
0
-0.01
0
10
20
30
40
50
60

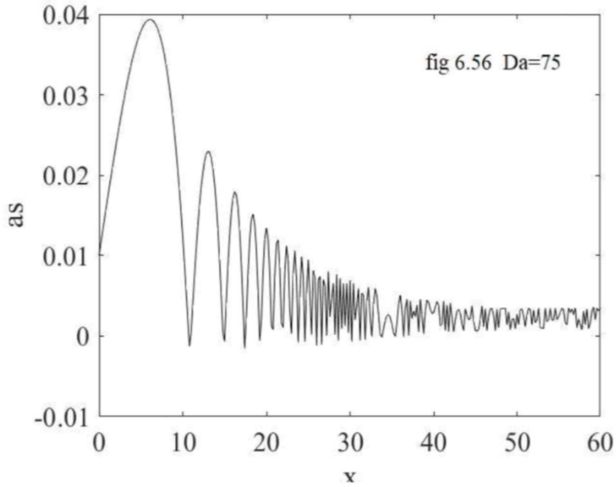


fig 6.56 Da=75
as
x
0.04
0.03
0.02
0.01
0
-0.01
0
10
20
30
40
50
60

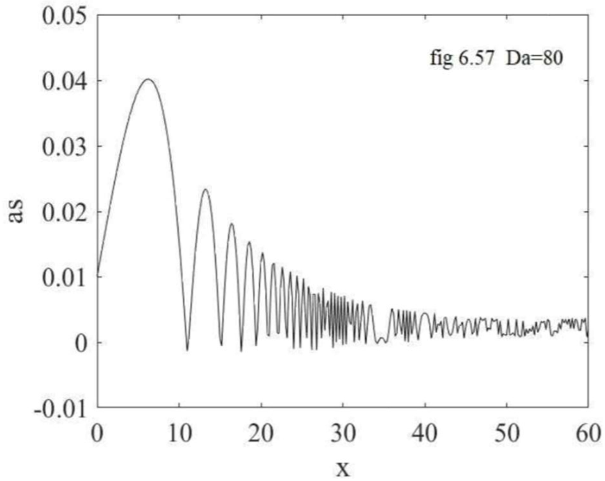


fig 6.57 Da=80
as
x
0.05
0.04
0.03
0.02
0.01
0
-0.01
0
10
20
30
40
50
60

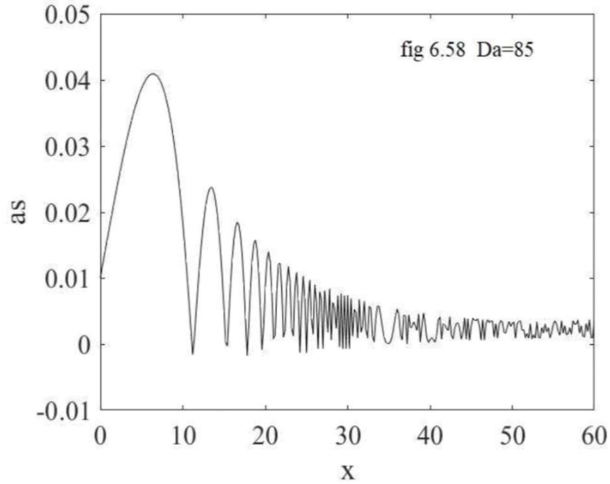


fig 6.58 Da=85
as
x
0.05
0.04
0.03
0.02
0.01
0
-0.01
0
10
20
30
40
50
60

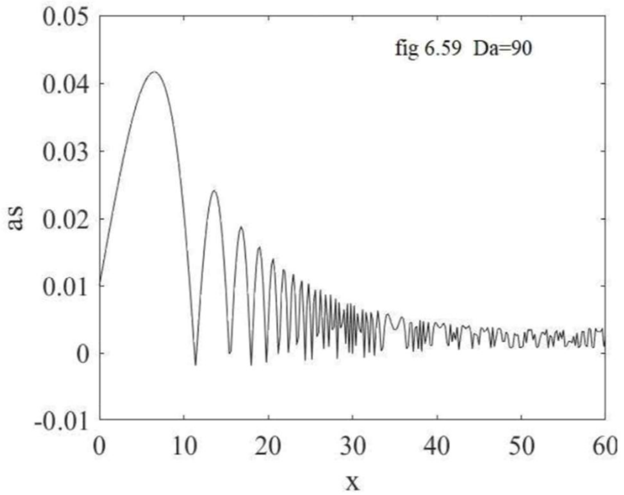


fig 6.59 Da=90
as
x
0.05
0.04
0.03
0.02
0.01
0
-0.01
0
10
20
30
40
50
60

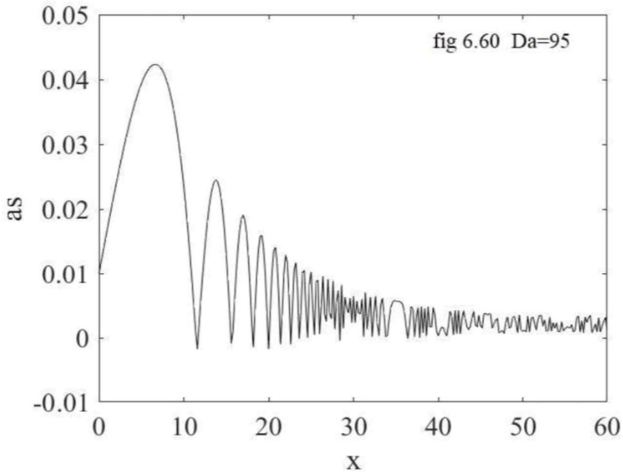


fig 6.60 Da=95
as
x
0.05
0.04
0.03
0.02
0.01
0
-0.01
0
10
20
30
40
50
60

The steady-state($a_s(x)$) is plotted for different values of D_a from 1 to 100, keeping other parameters constant at, D_b=0.6, d=0.2, f=1.4, q=0.002, e=0.01.

For fig 6.1, Da=1, first the amplitude of oscillations increases up to x=15 and after that, it shows damped oscillation. The peak value of a_s is smaller than 0.04.

For fig 6.2, Da=1.1, the plot is similar to fig 6.1, with a peak value approximately equal to 0.04.

For fig 6.3, Da=1.2, and the plot is similar to fig 6.1, with a peak value approximately equal 0.03.

For fig 6.4, Da=1.3, the amplitude of oscillations increases up to x=15 and then it decreases suddenly. After x=20 again, the amplitude increases till x=42, then it decreases suddenly.

For fig 6.5, Da=1.4, the amplitude of oscillation first increases up to x=12, then it decreases. Again, after x=20, the amplitude increases till x=35. After this, the oscillations are damped.

For fig 6.6, Da=1.5, the amplitude of oscillations increases up to x=10. After this, it continuously decreases.

For fig 6.7, Da=1.6, the plot is similar to fig 6.4, with a peak value of around 0.06.

For fig 6.8, Da=1.7, the amplitude of oscillation first increases up to x=15, then it decreases. Again, after x=20, the amplitude increases till x=40. After this the oscillations are damped.

For fig 6.9, Da=1.8, first the amplitude of oscillations increases up to x=15 and after that it shows damped oscillation. The peak value of a_s is approximately equal to 0.025.

For fig 6.10, Da=1.9, first the amplitude of oscillations increases up to x=12 and after that it shows damped oscillation. The peak value of a_s is approximately equal to 0.025.

For fig 6.10a, Da=2, first the amplitude of oscillations increases up to x=12 and after that it shows damped oscillation. The peak value of a_s is approximately equal to 0.03.

For fig 6.11, Da=2.1, first the amplitude of oscillations increases up to x=12 and after that it shows damped oscillation. The peak value of a_s is approximately equal to 0.025.

For fig 6.12, Da=2.2, first the amplitude of oscillations increases up to x=12 and after that it decreases suddenly. Again, after x=20 the amplitude increases till x=40 and then it decreases suddenly.

For fig 6.13, Da=2.3, first the amplitude of oscillations increases up to x=12 and after that, it shows damped oscillation. The peak value of a_s is approximately equal to 0.03.

For fig 6.14, Da=2.4, the amplitude of oscillation first increases up to x=15, then it decreases. Again, after x=20, the amplitude increases till x=35. After this, the oscillations are damped.

For fig 6.15, Da=2.6, first the amplitude of oscillations increases up to x=10 and after that, it shows damped oscillation. The peak value of a_s is approximately equal to 0.025.

For fig 6.16, Da=2.9, first the amplitude of oscillations increases up to x=10 and after that it shows damped oscillation. The peak value of a_s is approximately equal to 0.025.

For fig 6.17, Da=3, the amplitude of oscillation first increases up to x=15, then it decreases. Again, after x=20, the amplitude increases till x=40 and then it decreases suddenly.

For fig 6.18, Da=3.1, the amplitude of oscillation first increases up to x=15, then it decreases. Again, after x=20, the amplitude increases till x=35. After this, the oscillations are damped.

For fig 6.19, Da=3.2, the amplitude of oscillation first increases up to x=15, then it decreases continuously. The peak value of a_s is around 0.03.

For fig 6.20, Da=3.3, the amplitude of oscillation first increases up to x=15, then it decreases continuously. The peak value of a_s is around 0.02.

For fig 6.21, Da=3.4, the amplitude of oscillation first increases up to x=10, then it decreases. Again, the amplitude increases till x=30. After this the oscillations are damped.

For fig 6.22, Da=3.6, the plot shows damped oscillations after x=10.

For fig 6.23, Da=3.7, first the amplitude of oscillations increases up to x=10 and after that it shows damped oscillation. The peak value of a_s is approximately equal to 0.03.

For fig 6.24, Da=3.8 the amplitude of oscillation first increases up to x=10, then it decreases. Again, after x=20, the amplitude increases till x=35. After this the oscillations are damped.
For fig 6.25, Da=3.9 the plot is similar to fig 6.23.

For fig 6.26, Da=4, first the amplitude of oscillations increases up to x=12 and after that it shows damped oscillation. The peak value of a_s is approximately equal to 0.025.

For fig 6.27, Da=4.1, the amplitude shows an aperiodic increase and decrease.

For fig 6.28, Da=4.3, the amplitude of oscillation first increases up to x=10, then it decreases. Again, after x=20, the amplitude increases till x=35. After this the oscillations are damped.

For fig 6.29, Da=4.4, the amplitude of oscillation shows random increase and decrease.

For fig 6.30, Da=4.5, the amplitude of oscillation increases from x=15 till x=35 then the oscillations are damped.

For fig 6.31, Da=4.6, the amplitude of oscillation shows the random increase and decrease.

For figs 6.32, Da=4.7, the amplitude of oscillation decreases continuously.
For figs 6.33, Da=4.8, the amplitude of oscillation decreases and increases continuously.
For figs 6.34, Da=4.9, the amplitude of oscillation decreases continuously.
For figs 6.35, Da=5, the amplitude of oscillation decreases continuously.

For fig 6.36, Da=6, first the amplitude of oscillations increases up to x=8 and after that it shows damped oscillation. The peak value of a_s is approximately equal to 0.02.
For fig 6.37 Da=7, the amplitude of oscillation decreases continuously after x=30.
For fig 6.38 Da=9, the amplitude of oscillation increases and decreases continuously.

For figs 6.39,Da=10, the amplitude of oscillation decreases continuously after x=20.
For figs 6.40 to 6.60 , the amplitude of oscillation decreases continuously that is the oscillations are damped.

CONCLUSION

From the results of part 1, it can be observed that the values of steady-state are sensitive to initial conditions (y0). From the result of part 2, that is, variation of growth rate vs. wavenumber, it can be observed that the sign of growth rate of component ‘a’ depends upon the steady-state and the wavenumber. For component ‘b’, the growth rate is negative for all values of wavenumber.
From results of part 3 that, is variation of steady-state vs Da it can be observed that up to D_a=10, the pattern of oscillation of a_s was changing with respect to D_a. But for values of Da>10, the pattern of oscillations is the same and only the amplitude of oscillations changes with Da.
These results can help in understanding the stability in reaction diffusion system with Oregonator model.
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Appendix

MATLAB code

```
%Function for solving the steady state
function F= bz_rkn(x,Y)
   D_b=0.6;
   d=0.2;
   D_a=1;
   f=1.4;
   q=0.002;
   e=0.01;
  % Equations 12-15
   F(1,1)=Y(2);
   F(2,1)=-(d^2/(e*D_a))*(Y(1)-Y(1)^2 -
(f/(Y(1)+q))*(Y(1)*Y(3)-q*Y(3)));
   F(3,1)=Y(4);
   F(4,1)=(Y(3)-Y(1))*d^2/D_b;
end
```

Use this function in ode45 solver to get the SS solution.

```
y0= [0.01,-0.0007,0.01, -0.00010]; % for different y0
different steady state is plotted
% taking x =0:0.2:60
[xsol,Ysol]=ode45(@bz_rkn,[0:0.2:60],y0);
plot(xsol,Ysol(:,1),'k')
xlabel('x');
ylabel('as');
ax=gca;
ax.FontSize=17;
ax.FontName='Times New Roman';
```

After getting a_s and b_s beta vs k is plotted.

```
D_b=0.6;
d=0.2;
D_a=1;
f=1.4;
q=0.002;
e=0.01;
as=Ysol(151,1);%change index to get a plot for different
values of x
bs=Ysol(151,3);
k=[0:0.01:1000];
beta=-k.^2.*D_a/d^2+(1-2*as)/e-f/e*(as+bs-q)/(as+q)-
f/e*bs*(as-q)/(as+q)^2;
plot(k,beta,'k')
```