PHYS 7123 FALL 2003 Igor Romanovsky
Statistical mechanics II

Course project description plan

I have decided to consider the problem of scattering of electrons in a quantum dot. Later I had to change my task and consider the probem of particles bouncing between the wasboard walls. At first couple words about what quandum dots are. Quantum dots are low-dimensional nanometer-sized man-made systems where a few electrons can be confined. Usually quantum dots are fabricated by restricting the two dimensional (2D) electron gas in a semiconductor heterostructures laterally by voltage, applied to electrostatic gates or by etching techniques. There are usually two top gates that create two tunnel barriers.

One possible way to model quantum dot is by a two-wall potential

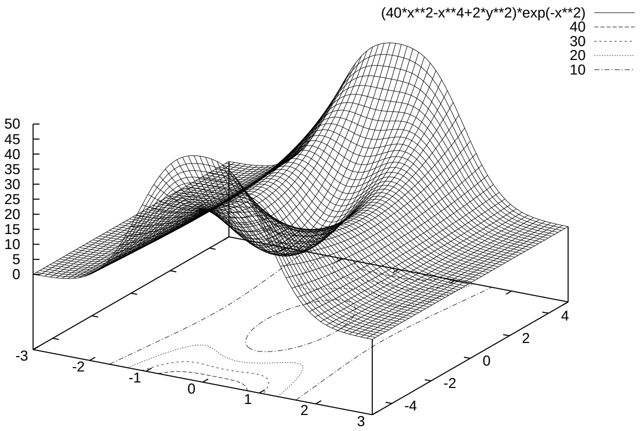

Figure 1: The “soft walls” model potential for quantum dot.

$$V(x,y) = (ax^2 - bx^4 + cy^2)\exp(-x^2) \tag{1}$$

where $a, b, c > 0$ are some constants.
The other possible way to model quantum dot is to take open 2D stadium with hard walls and consider the ball (electron) bouncing in the space between these walls. The walls of the stadium can be taken in the form

$$y = \pm\sqrt{-Ax^2 + Bx^4 + C} \tag{2}$$

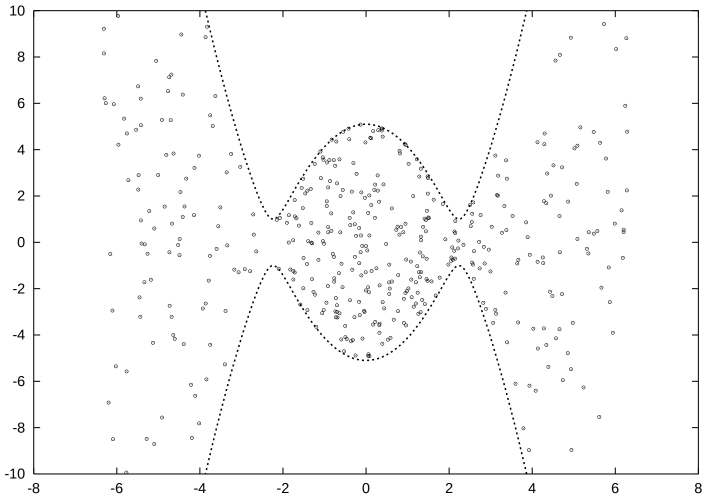

Figure 2: The "hard walls" model potential for quantum dot. I used this potential in my project.

where A , B ,C > 0 are again some constants that are the parameters of the system. (y_0 is the width of the two "necks of the bottle" through which electron can penetrate or escape.) This problem with can be viewed as a problem of a molecule diffusing through a small pore (however pores are usually three dimensional). Since billiards are easier to consider, I take the second model for my calculations (hovewer may be it is possible to consider both cases). Although it is clear that the problem of scattering and diffusion of electrons through this system should be solved involving quantum mechanics, and interactions between particles in the same quantum dot should not be totally neglected and that soft wall potential is better than hard wall poential, I expect that the classical description of the one particle in external potential like this can give results that are close to reasonable .

The goals of this project:

Study the dymamics of the particle in the dot, plot Poincare sections, investigate the system using the periodic orbit theory, find the diffusion coefficient and escape rate of electrons from the dot.

The schedule of the project:

- **Thu Oct 23 2003 :** The simulator for the particle, bouncing in the cavity of the dot will be written. The Poincare sections will be calculated and drawn.

- **Thu Oct 30 2003 :** The Jacobian of the system will be found. The first several prime cycles will be found and stabilities will be calculated for them.
- **Thu Nov 06 2003 :** The program will be revized to eliminate numerous bugs. The escape rate will be calculated primitively (in order to compare it later with result given by periodic orbit theory)
- **Thu Nov 13 2003 :** Hopefully, the escape rate and diffusion coefficient for the quantum dot will be found (using dynamical zeta function).
- **Thu Nov 20 2003:** The crude estimate of diffusion coefficient and escape rate will be found and compared to those obtained earlier. The graphs, showing dependence of diffusion coefficient and escape rate on the parameters of the system α , β , y_0 will be made.
- **Thu Nov 27 2003:** The programs will be rewritten again to half the number of the bugs. Errors will to be corrected and crude draft of report will be prepared , the results of caculations will be analyzed. I will try to use Gutzwiller formula to find the spectrum of energy levels of electron in the cavity.
- **Thu Dec 4 2003:** The project will be polished to eliminate errors and resolve problems.
- **Thu Dec 11 2003:** Term paper deadline.

(Stage 1) The code of the FORTRAN program that simulates the particle bouncing in the quantum dot has been written (the text of the program is given in the end of this file). The results of simulation are represented by figures 3,4,5 The program finds precisely trajectories of the particles and plots Poincare section.

I implemented the safest possible way to find the points of intersection of trajectories with the walls of the dot:

a) at first stage the particle is approached to the vicinity of the wall.

b) then the minimization subroutine is used to move the particle very close to the wall.

c) the point of intersection is found with great accuracy by Newton method.

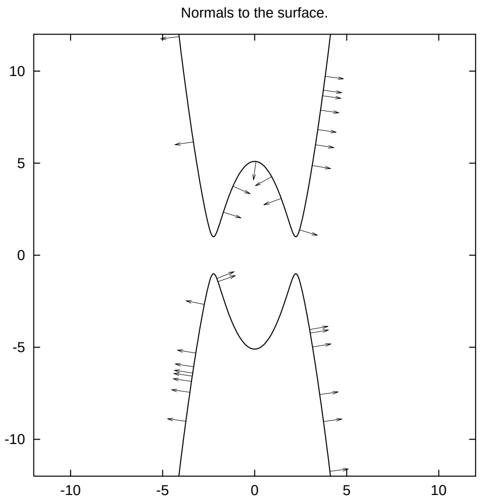

Figure 3: In order to simulate reflections of the particles from the walls I had to find the intersections of trajectories with the walls of the dot and find the outward normals in the points of collision.

(Stage 2) Subroutines for calculating the Jacobian matrices were added to the FORTRAN program. I am going to use them later to find the. Stabilities of periodic orbits. The stability matrix for our problem is equal to

$$\mathbf{J}_p = (-1)^{n_p} \prod_{k=n_p}^{1} \begin{pmatrix} 1 & L_k \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ R_k & 1 \end{pmatrix} \tag{3}$$

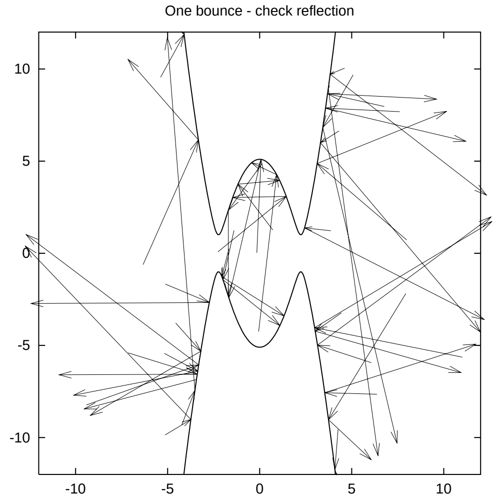

Figure 4: This picture shows how particles reflect from the walls. One bounce only shown for clarity.

where

$$L_k = \sqrt{(x_k - x_{k-1})^2 + (y_k - y_{k-1})^2} \tag{4}$$

is the length of the kth segment of the trarajectory between collisions (we assume that the velocity of the particle V=1) and

$$R_k = 2\frac{C_k}{\cos(\phi_k)} \tag{5}$$

C_k - is the local curvature in the point of collision that followed the free flight. In general case the curvature of the line $y = f(x)$ is given by

$$C_k = \frac{f''(x_k)}{(1 + (f'(x_k))^2)^{3/2}} \tag{6}$$

Now I want to say couple of words about cycles. The first several shortest cycles is easy to find (Figs..).

But problem arises when we try to find longer cycles. The concave part of the dot is the generator of these problems. Unlike for convex part, the concave part of the dot makes it possible for particle to reflect many times from walls withing concave part. It is even possible that there are trajectories in the system that almost tangent to the surface in the concave region. On the other hand it is impossible to build a cycle such that all points of it belong to the same concave part

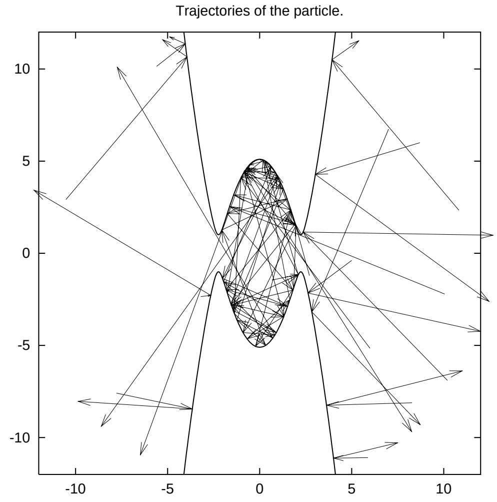

Figure 5: The "The trajectories of the particle bouncing in the quantum dot. This picture was produced by the simulator.

In other words the symbolic dynamics of the particle that moves in the potential of the dot is different from the symbolic dynamics for the particle that bounces from the, say four disks.

I think the Newton-Rapson method will not work well in our case, we must use variational methods to find closed trajectories, and it means that we must distinguish different trajectories and we must know exactly what cycle can exist to be able to start looking for it. That is we need to build symbolic dynamics for our system. At first I tried to implement very simple symbolic dynamics. I considered the fundamental domain of the washboard walls. I gave symbol to every wall of the fundamental domain. For, example, the x axis was given symbol "0" , y axis was given symbol "3" and the hole line was given symbol "3". The curved part of the dot was split into two parts. The convex part was labeled by "1" and concave part was labelaed "2". I naively thought that my symbolic dynamics was good. In fact it was not true. The concave part of the billiard is the droplet of poison that makes the problem of finding symbolic dynamics very difficult. I was given references to several papers which described symbolic dynamics of the similar systems. Only then I realized how difficult my problem is.

I wrote the program that generates special words of symbols. Each word, generated by this program can be associated to some trajectory, but some of this trajectories are forbidden so, at least we can plug the word into the routine that extremizes the action of the possible trajectory and see what happens to

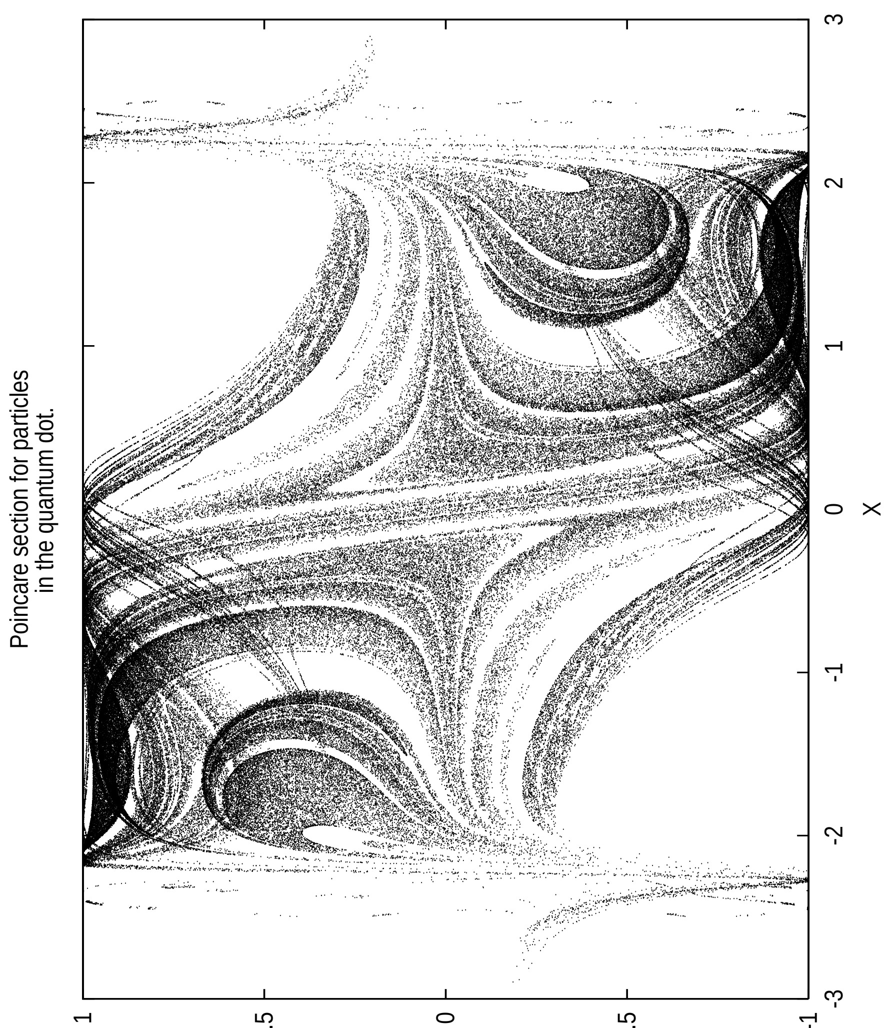

Figure 6: The Poincare section for the particle bouncing in the dot. Actually this picture is made for particles that have survived at least six bounces with the walls. This plot shows the X component of velocity of the particle in the moment just after collision versus the X coordinate of the point of collision.

it. With great probability, I think, the extremization process will result with something reasonable. But if as an outcome we get something bad we should just ignore such result. In other words, despite all my attempts I still have very vague notion about what kind of pruning rules exist in the system. Now I am working at the extremization routine to make it understand the symbols generated by the first program. Unfortunately despite all attempts the second program refuses to work. So this is the place where I am now at this time. And I think that I will not be able to finish this problem to the end of the semester.

References.

[1] J.D.Meiss 'Symplectic maps, variational principles, and transport.' Rev.Mod.Phys., Vol. 64, No.3, July 1992

[2] E.E. Narimanov and A. Douglas Stone 'Theory of the periodic orbits of a chaotic quantum well.' Phys.Rev.B V57, 16 , April 1998

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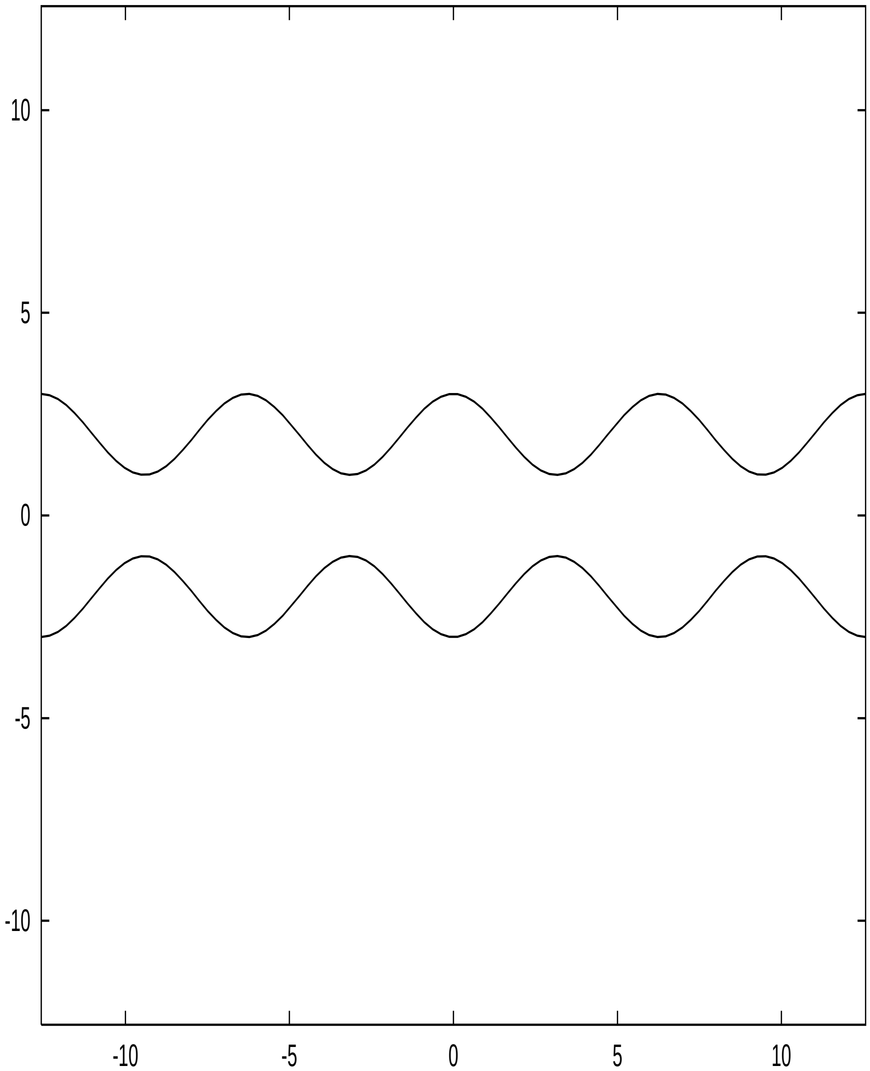

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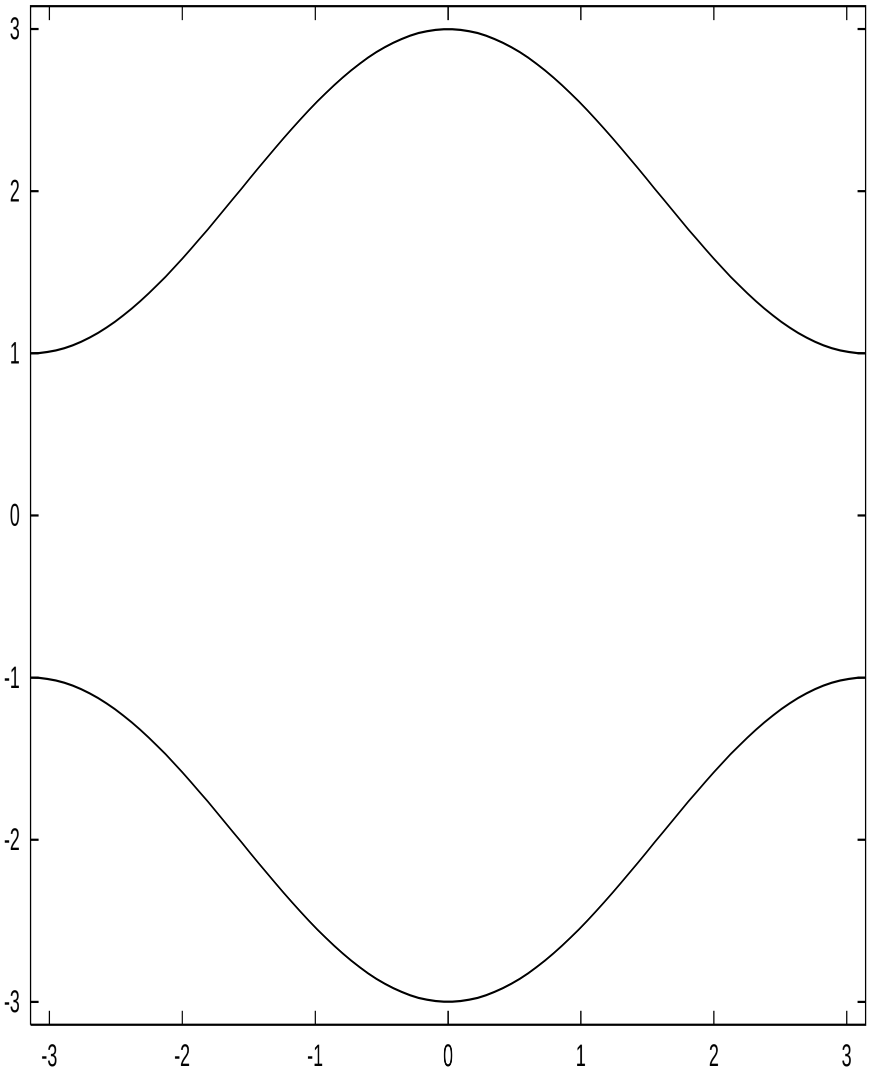

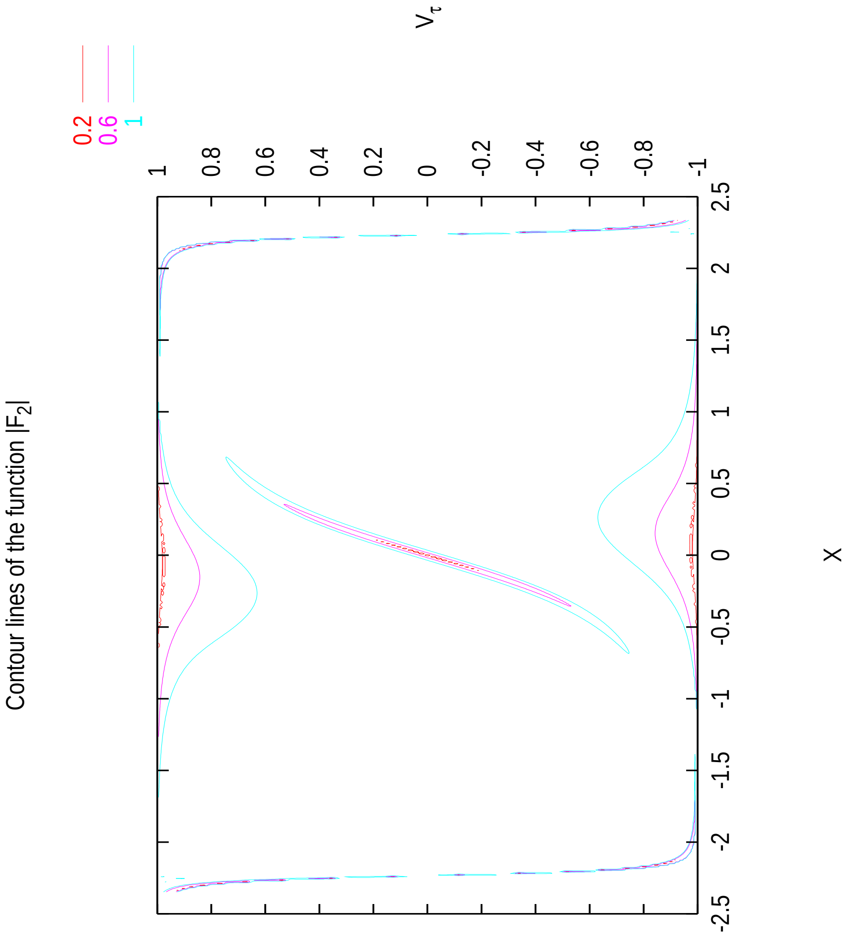

Figure 7: The level lines of the function $||F_2(\mathbf{x})|| = ||f_2(\mathbf{x}) - \mathbf{x}||$ Where $\mathbf{x} = (x, v_\tau)^T$ with v_τ - component of velocity, parallel to the surface at the point of collision. $f_2(\mathbf{x})$ is our map function, (that corresponds to the transformation $f(\mathbf{x})$-'leap-bounce' applied two times to the initial point on the surface inside the dot). The norm $||\ \mathbf{x}\ ||$ is defined as $||\ \mathbf{x}\ || = \sqrt{x^2 + v_\tau^2}$ and , therefore, for the particles that fly away after one bounce this norm is infinite $||\ F_2(\mathbf{x})\ || \to \infty$ but in the vicinity of periodic orbits with period $N = 2$ this norm should approach zero $||\ F_2(\mathbf{x})\ || \to 0$.

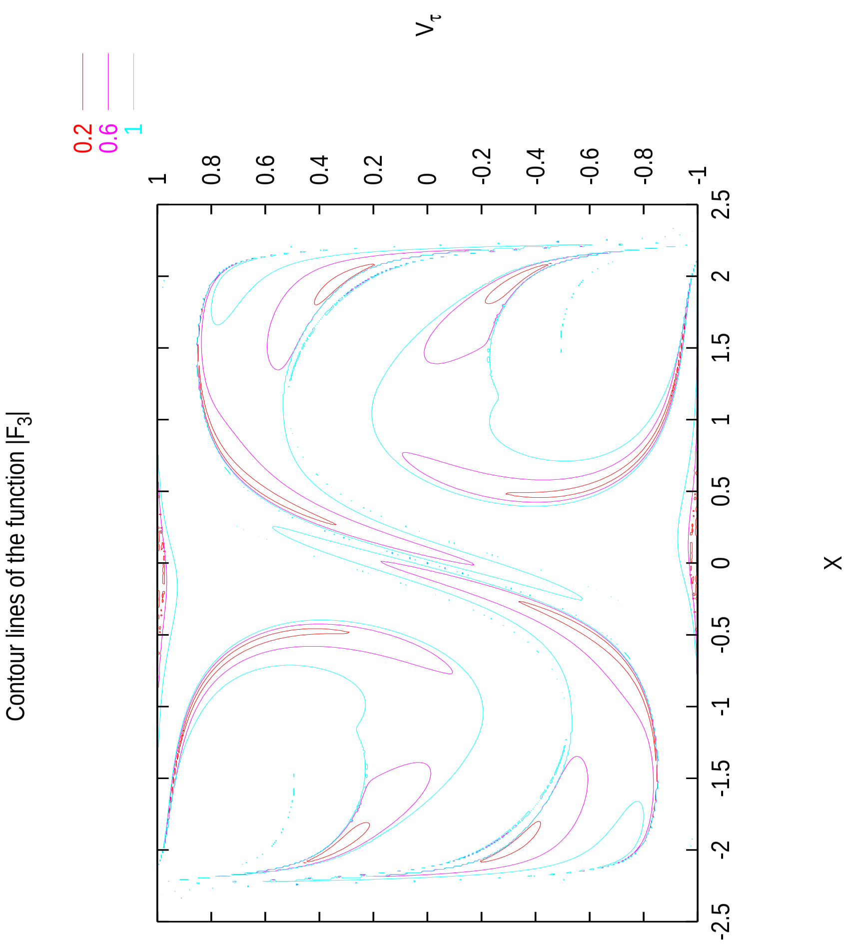

Figure 8: The level lines of the function $||F_3(\mathbf{x})|| = ||f_3(\mathbf{x}) - \mathbf{x}||$. Read more detailed explanation in the caption to the previous figure.

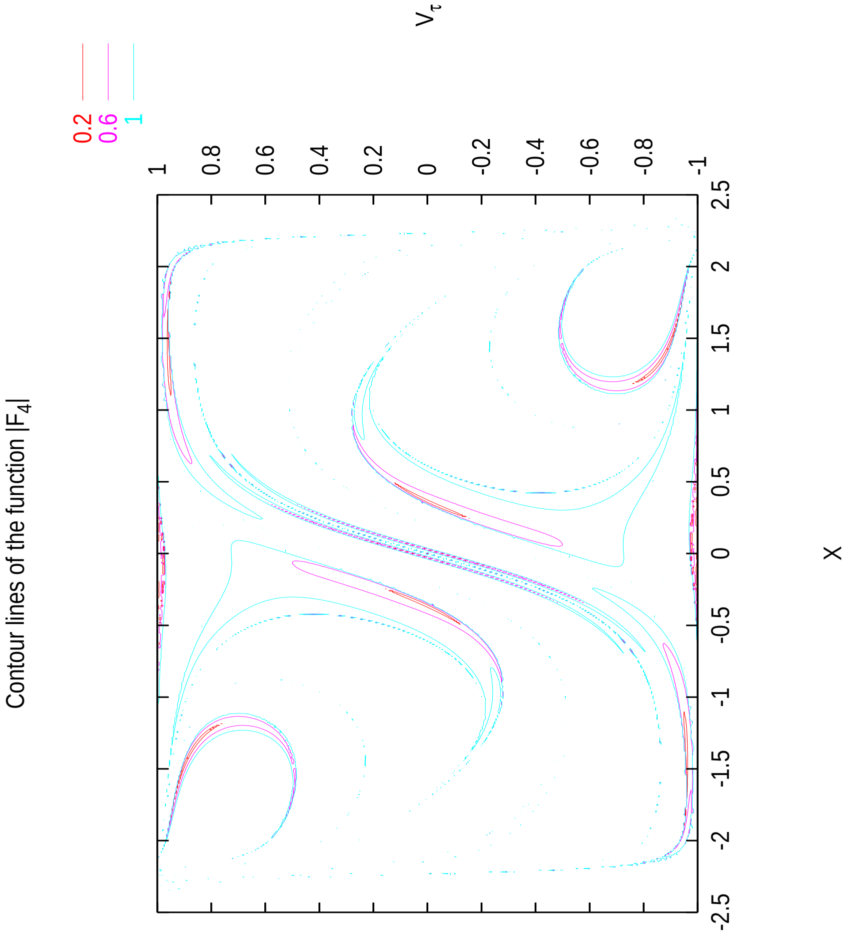

Figure 9: The level lines of the function $||F_4(\mathbf{x})|| = ||f_4(\mathbf{x}) - \mathbf{x}||$. Read more detailed explanation in the caption to the figure 7. I should note however that the function $||F_4(\mathbf{x})||$ is already so sharp that it is almost impossible to draw the picture well enough to show adequately the regions where it is small. These regions become very narrow, which means that it is very difficult task to find all zeroes of $F_4(\mathbf{x})$ by Newton Raphson method.

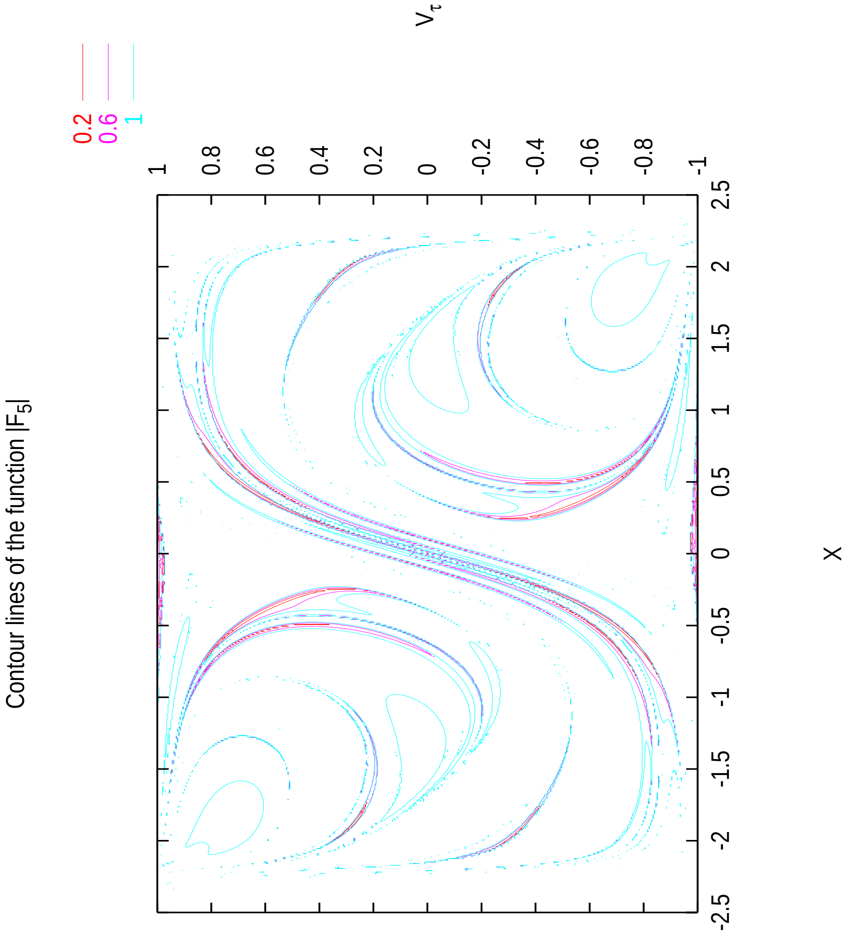

Figure 10: The level lines of the function $||F_5(\mathbf{x})|| = ||f_5(\mathbf{x}) - \mathbf{x}||$. Read more detailed explanation in the caption to the figure 7 and in the caption to previous picture.