Particles in a trigonometric potential: a brief discussion of the numerical approach in the study of nonintegrable hamiltonian dynamical systems

Cristian-Constantin Lalescu

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Contents

1 Introduction

The purpose of this work is to bring together several theoretical concepts and apply them to a concrete example. In the context of chaotic dynamical systems, numerically simulated trajectories are analyzed to find invariant sets in the phase space (for the specific system), and also to find displays of diffusion or strange diffusion.

The physical system being studied is that of particles moving in a plane, under the influence of a trigonometric potential $V(x, y) = A_x \cos x + A_y \cos y + B \cos x \cos y$. For each particle, the Hamiltonian is:

$$H(x, y, p_x, p_y) = \frac{1}{2}(p_x^2 + p_y^2) + V(x, y) \tag{1}$$

Several values for the constants $A_{x,y}$ and B make for several shapes of the potential, and generate different dynamical systems. Note first that this is a conservative system; and second that we are working with dimensionless quantities.

Generally the system is not integrable, however if $B = 0$ or $A_x = A_y = 0$ the equations of motion become separable and they may be solved (the system is a simple superposition of two gravitational pendulums). This can be shown as follows (note that it is more straightforward to use Newton's equations for this proof):

Case 1 $B = 0$

$$V(x,y) = A_x \cos x + A_y \cos y \tag{2}$$

Newton's equation's will be:

$$\begin{cases} \dfrac{d^2x}{dt^2} = A_x \sin x \\ \dfrac{d^2y}{dt^2} = A_y \sin y \end{cases} \tag{3}$$

Case 2 $A_x = 0,\ A_y = 0$

$$V(x,y) = B \cos x \cos y \tag{4}$$

Newton's equations will be:

$$\begin{cases} \dfrac{d^2x}{dt^2} = B \sin x \cos y \\ \dfrac{d^2y}{dt^2} = B \cos x \sin y \end{cases} \tag{5}$$

which are equivalent to

$$\begin{cases} \dfrac{d^2}{dt^2}(x+y) = B \sin(x+y) \\ \dfrac{d^2}{dt^2}(x-y) = B \sin(x-y) \end{cases} \tag{6}$$

Another fact that may be immediately deduced is that if a particle's energy is very large, it will move almost without "feeling" the external potential. A very large energy would imply that the potential energy is negligible next to the kinetic energy, so the system would be very close to that of a free particle moving in a plane.

However, in a large enough domain of energies for the particle (determined by the constants $A_{x,y}$ and B), chaotic behaviour may be observed.

To characterize the system, we may look at Poincaré sections, and we may attempt to connect these with the study of diffusion (or strange diffusion). As stated above, the purpose of this work is not to characterize this dynamical system, but just to briefly touch on some possibilities of study. The numerical method used here for the time evolution of the system is the "classical" fourth order Runge-Kutta method. Generally this is not an acceptable method for this particular type of study, as the Runge-Kutta methods do not usually preserve the symplectic invariants. Proper methods have however been developed [1], and they may be employed with relative ease.

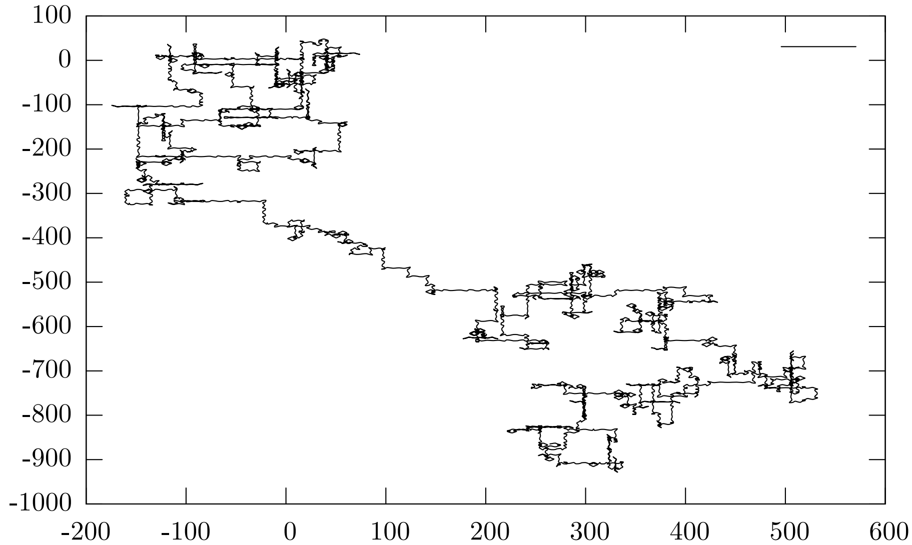


Figure 1: Trajectory of a particle in the chaotic regime. The parameters of the potential are $A_x = 1, A_y = 1, B = 1$, the energy of the particle is 1, and the time interval is 10^4.

Note that the code used here for the time evolution was written in C++, with the specific purpose of being able to easily simulate any system with a "reasonable" amount of degrees of freedom, with any numerical method that the user sees fit to use (that needs to be written first however).

Before moving on, we will note that

$$H(x, y, p_x, p_y) = H(x(\text{mod}2\pi), y(\text{mod}2\pi), p_x, p_y) \tag{7}$$

and obviously this symmetry also holds for the equations of motion.

2 Poincaré sections

For this "simple" system with only two degrees of freedom, Poincaré sections are easy to work with. Briefly, they give a first idea of what the trajectories (in phase space) look like — for a rigurous introduction in the subject, see [2].

If we define the Hamiltonian flow induced by temporal evolution on the phase space:

$$\phi^t(x(0), y(0), p_x(0), p_y(0)) \equiv (x(t), y(t), p_x(t), p_y(t)) \tag{8}$$

we can more explicitly say that Poincaré sections let us find the sets $\mathcal{M}$ that are invariant to ϕ (note that in the above equation x, y, p_x, p_y are solutions to the equations of motion, not variables):

$$\phi^t(\mathcal{M}) = \mathcal{M}\ \forall t \tag{9}$$

Taking into account the periodicity of the equations, we will look at trajectories only for $(x, y) \in (0, 2\pi) \times (0, 2\pi)$, so a portion of the phase space: $(0, 2\pi) \times (0, 2\pi) \times \mathbb{R} \times \mathbb{R}$ (all of the trajectories will be "brought back" to this domain by the transformation ($x \longrightarrow x \mod 2\pi$) and similar for y).

Let $(\tilde{x}(t), \tilde{y}(t), \tilde{p}_x(t), \tilde{p}_y(t)) \equiv \gamma(t)$ be a trajectory. For all times τ_i such that $\tilde{y}(\tau_i) = y_0$, we will "collect" $\tilde{x}(\tau_i)$ and $\tilde{p}_x(\tau_i)$. Note that if we have these three values, we can immediately find p_y^2, so we have the complete state of the system (still lacking the sign of p_y, but that is not essential). If we name $T_\eta(\gamma) = \{(\tilde{x}(\tau_i), \tilde{p}_x(\tau_i))\big|\forall\tau_i \in \mathbb{R}$ such that $\tilde{y}(\tau_i) = \eta\}$, then we are sure that $\mathcal{T} = \cup_{\eta\in[0,2\pi)}\overline{T_\eta}$ is an invariant set for ϕ (the bar denotes closure). By construction this set contains the entire trajectories for finite times, and the closure was taken to insure that the limits for infinite times are also in the set — so by construction the set is invariant.

$\mathcal{T}$ is invariant to ϕ, but we only need a T_{y_0} to get the general idea of its structure. We will define

$$\varphi_E(x, p_x) = (\hat{x}, \hat{p}_x) \tag{10}$$

such that if we have a particle with energy E leaving from $(x, y_0, p_x, \sqrt{p_y^2})$, and the solution of the equations of motion is $(x(t), y(t), p_x(t), p_y(t))$, then $(\hat{x}, \hat{p}_x) = (x(\tau), p_x(\tau))$, where $\tau = \min\{t > 0\big|y(t) \mod 2\pi = y_0\}$.

The Poincaré section (PS) is generally the surface obtained in phase-space by fixing one of the coordinates. If the system is conservative, than the momentum associated to the fixed coordinate may be "ignored" also, as it will have at most two possible values for each point (to put it more rigorously, we intersect this section with the surface of constant energy, and we are looking at the dimension of the sets). As described before, the PS helps give an idea of what the invariant sets of the phase space are — we will be interested in looking at all the invariant sets for a given value of the energy.

Note that if the equations are separable, than we find that

$$H(x, y, p_x, p_y) = H_1(x, p_x) + H_2(y, p_y) \tag{11}$$

and the energy for each degree of freedom will be fixed. This means that the trajectories will be found on a two-dimensional surface (once we fix the total energy, then the energy for one of the degrees of freedom — we have two globally conserved quantities), so generally their intersection with the PS $y = y_0$ will be found on a one-dimensional manifold. Note however that this is only true in the case of quasiperiodicity, and that it is possible that the invariant sets associated to a trajectory are just finite sets of points — in the case of coincidence of frequencies for the two degrees of freedom. For the nonlinear system studied here, this will most likely not be the case.

Whenever we find one-dimensional invariant sets in the PS, we will say that quasiperiodicity has been observed. As for the two dimensional invariant sets, we will say that they are "areas" of chaotic behaviour. Generally areas of quasiperiodicity are referred to as islands.

Poincaré sections were computed for several sets of parameters for the potential, and for several values of the energy. To discuss the PS plots attached to this document (in the appendix), we will first note that each color is attached to a specific trajectory. That being said, it becomes very easy to distinguish between areas of quasiperiodicity or chaotic behaviour.

The first thing that a PS tells us is the way the invariant sets look. The second thing is found when we plot PS for several values of the energy: the sets change, and there are points where these changes are discontinuous — these are "bifurcations" points. If we see an invariant set as a "stable point" of φ, then it would probably be interesting to count the number of stable points for each value of the energy.

3 Diffusion and strange diffusion

If we think of what the trigonometric potential looks like, then we can say that the PS approach treats the problem from a "microscopic" perspective. "Macroscopically", we will look at scales at which the period of the potential is negligible, and we will look at the average behaviour of large sets of particles moving at random — we will look for diffusion and strange diffusion.

To be more specific, we will generate N "long" trajectories, and we will average (for each t) the quantities $(x(t)-x(0))^2, (y(t)-y(0))^2$ and their sums $r^2(t)$. Afterwards, we will look at

$$\langle r^2(t)\rangle = D_r t^{\alpha_r} \tag{12}$$

and similar quantities for each coordinate.

Normal diffusion is found if the exponent is $\alpha = 1$. Otherwise we are dealing with strange diffusion: subdiffusive regime ($\alpha \in (0,1)$), superdiffusive regime ($\alpha \in (1,2)$) or ballistic regime if $\alpha = 2$.

The natural idea in regards to these computation is to start from the origin with a lot of particles that leave in random directions. However, this will generally not give conclusive results, because when we speak of diffusion or strange diffusion, we speak of chaotic trajectories. Three things may happen to a particle: it can get "caught" around a minimum of the potential, it can move along a chaotic trajectory, or it can find a path in between the maximums of the potential, and move ballistically ("escape" the potential). If a particle has a chaotic trajectory, it will display both types of behaviour [3]. This is because chaotic trajectories tend to "stick" to quasiperiodic islands for long periods of time (this is why gradients of color may be observed in some of the PS plots).

A "good policy" for finding a diffusion coefficient, or the exponent of a strange diffusion regime, is to look at the PS sections, and start from points randomly distributed in the invariant set of points belonging to chaotic trajectories.

A dependency of the diffusion coefficient on the energy was expected, but tests were too few to give conclusive results — for these tests, the first "naive" approach was used. Note that the diffusion coefficient can only be defined for normal diffusion.

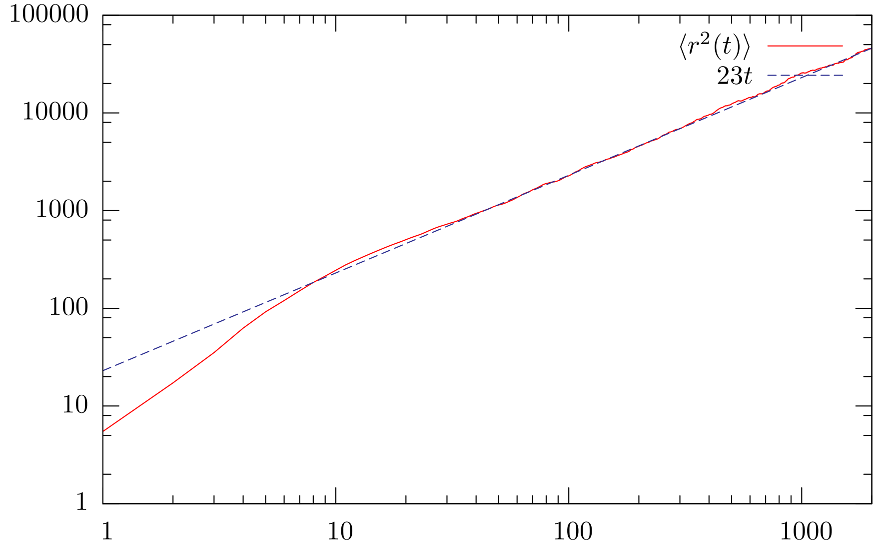


Figure 2: Normal diffusion. 300 trajectories, starting from (π, π) and randomly oriented momentum, for $A_x = A_y = B = 1$, an energy of 1.5, and a total time of 2000.

Normal diffusion was only studied for the above potential defined by $A_x = A_y = B = 1$, and for only three values of the energy:

E	$\langle x^{(}t)/t\rangle$	$\langle y^2(t)/t\rangle$	$\langle r^2(t)/t\rangle$
1.00	13	16	29
1.25	12	11	23
1.50	12	11	23

The diffusion coefficients were computed as averages over the second half of the time interval. The fact that the diffusion is not isotropic is the first sign that the results are not ideal. But from figure 2 we can see that what we are observing is diffusion, and the errors can not be very large. If accurate results were required, only more trajectories starting from points uniformly distributed in the chaotic area would be needed (note that for this case, the entire PS is one single chaotic region — this was the hint that this case gave normal diffusion).

As for superdiffusion, simulations were performed for three values of the energy in the case of $A_x = A_y = 1,\ B = 0.5$. It was trivial to estimate the

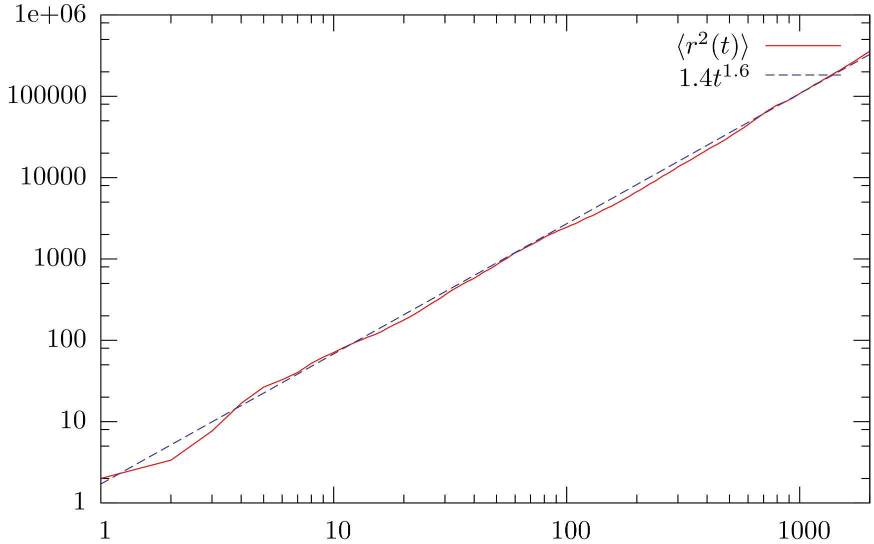


Figure 3: Super diffusion. 300 trajectories starting from points uniformly distributed in a rectangle in the chaotic area, for $A_x = A_y = 1,\ B = 0.5$, an energy of 0.75, and a total time of 2000.

exponent α just from plotting $\langle r^2(t)\rangle$ as a function of time, as in figure 3, no interpolation method was used for this problem — note however that it is always possible to find this exponent with the mean squared method. It is also relevant that due to the limited nature of this study — a time interval of 2000 is very small, in [3] the time intervals used to find the results presented were of $10^4 - 10^5$ — a direct estimate from the graph is probably as good as one computed with the proper statistical methods. For an energy of 0.5, the exponent is roughly 1.5, and for an energy of 1, it rises to 1.7 — note however that it is different for each coordinate. It was also confirmed that (see the PS for these parameters) the center island is one of ballistic movement along the second coordinate, as the top island is along the first coordinate.

4 Conclusions and perspectives

The actual work performed in order to gather these results consisted of two main points:

- writing a code ("from scratch") that would solve the equations of motion for a point particle (or any system with a reasonable number of degrees of freedom); writing the code that would compute the PS (actually, the intersections of the trajectories with the PS), and the statistics for the diffusion-strange diffusion study.

- running the simulations, and putting together the results.

The purpose of the work was to bring together several notions and methods that were studied in various contexts, and to experience how they should be used. The dynamical system that was studied, of particles moving in a trigonometric potential, proves to be very complex. As it can be seen from the PS that were computed, generally we can not find fully chaotic regimes, or fully quasiperiodic. This means that for most triplets (A_x, A_y, B) we will be dealing with the phenomena of strange diffusion. There are several steps for continuing the study:

- the numerical integrator needs to be replaced.
- for each PS, φ should be interpolated. The way the interpolation coefficients vary with the energy should be looked at.
- the case of $A_x, A_y \sim O(1)$ and $B << 1$ should be looked at more closely.
- statistics concerning diffusion and strange diffusion should be performed for a greater number of energies, to check how the trajectories tend to be ballistic as the energy increases. Also, it should be checked if there is a link between the surface areas of the islands of ballistic motion and the exponent of superdiffusion.

References

[1] Haruo Yoshida — *Construction of higher order symplectic integrators*, Physics Letters A, 1990

[2] V. I. Arnold — *Ordinary Differential Equations*, MIT Press, 1978

[3] J. Klafter and C. Zumofen — *Lévy statistics in a Hamiltonian system*, Physical Review E, 1994

5 Appendix: Poincaré section plots

Trajectories were simulated starting from points distributed in a rectangular grid (in some cases, for certain islands additional initial points were used). For all the plots presented, the fixed coordinate was $y = \pi$, but the data was collected for more values of y (this is useful to "truly" see what the invariant sets look like). As for the axis, the horizontal is along the x coordinate, and the vertical is along the momentum p_x.

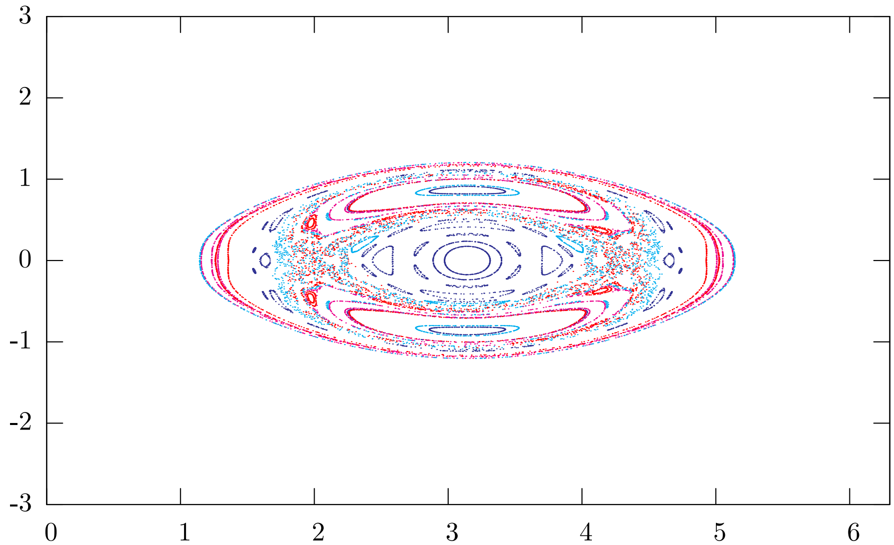


Figure 4: $A_x = 1,\ A_y = 1,\ B = 0.5,\ E = -0.75$

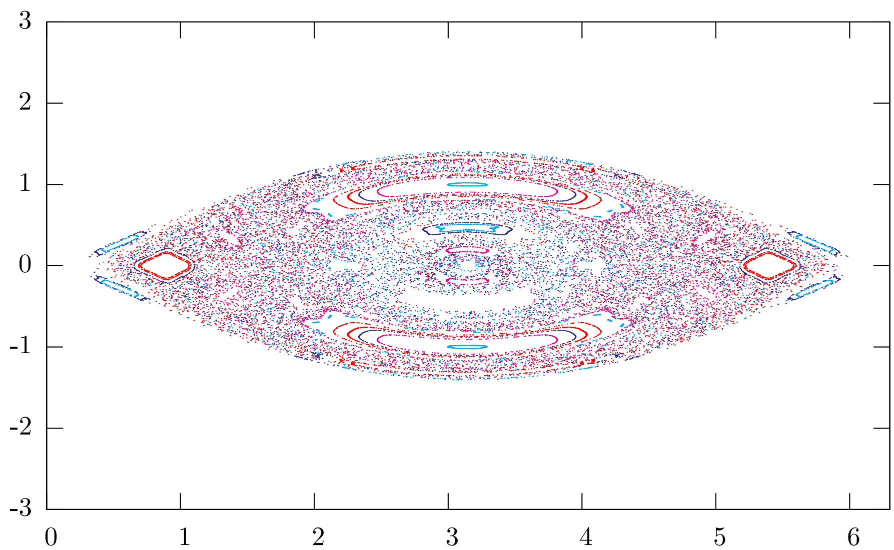


Figure 5: $A_x = 1,\ A_y = 1,\ B = 0.5,\ E = -0.50$

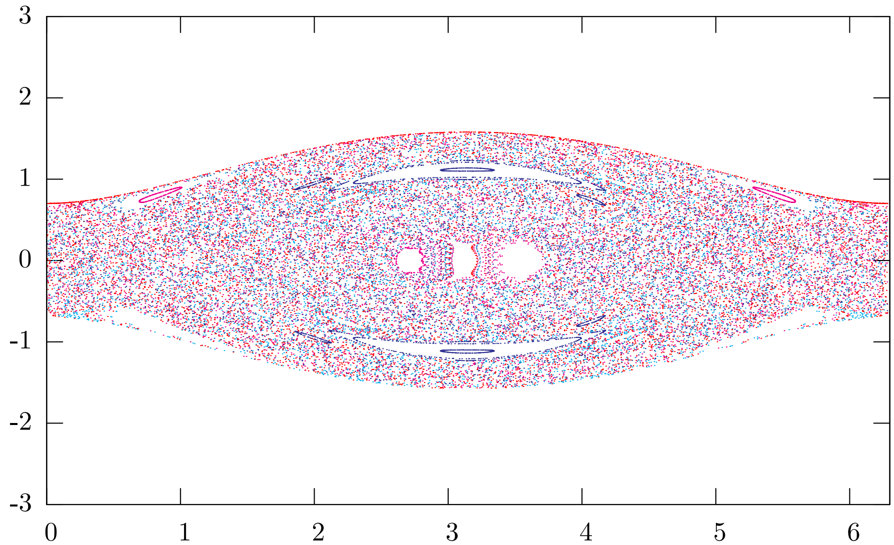


Figure 6: $A_x = 1,\ A_y = 1,\ B = 0.5,\ E = -0.25$

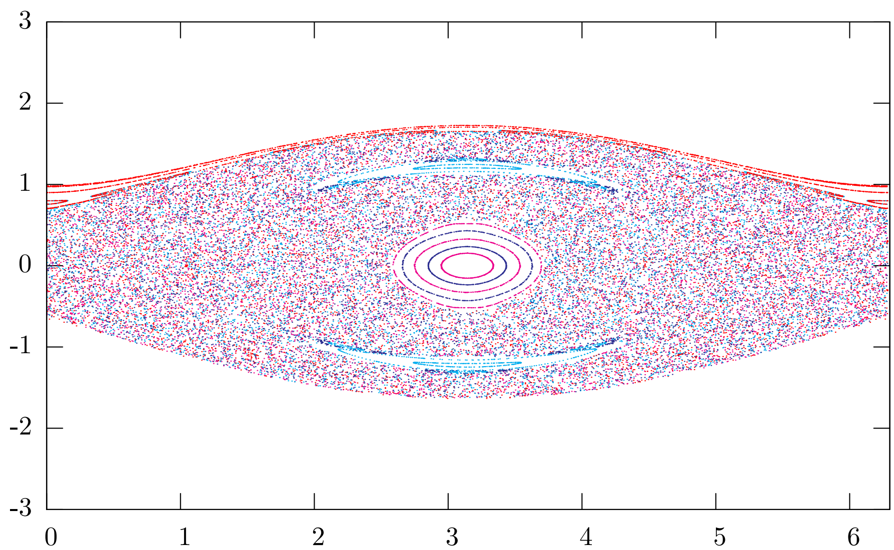


Figure 7: $A_x = 1,\ A_y = 1,\ B = 0.5,\ E = 0.00$

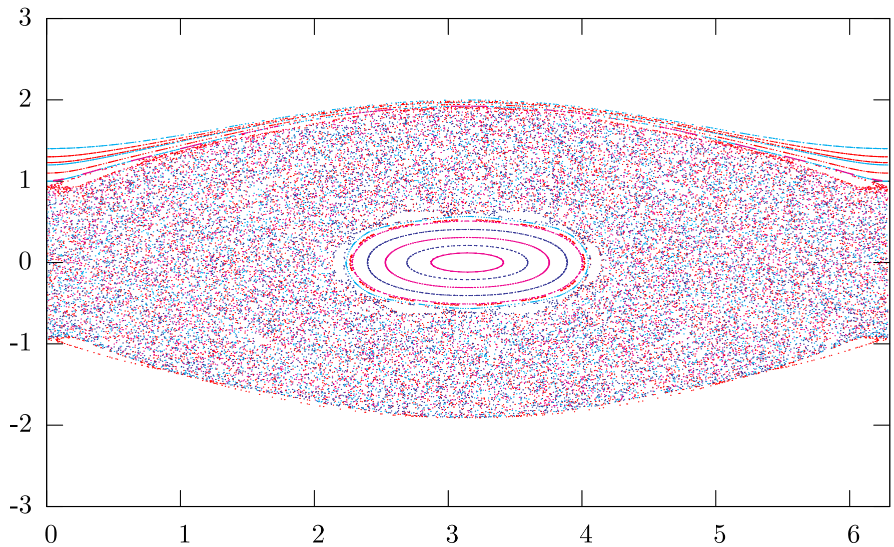


Figure 8: $A_x = 1,\ A_y = 1,\ B = 0.5,\ E = 0.50$

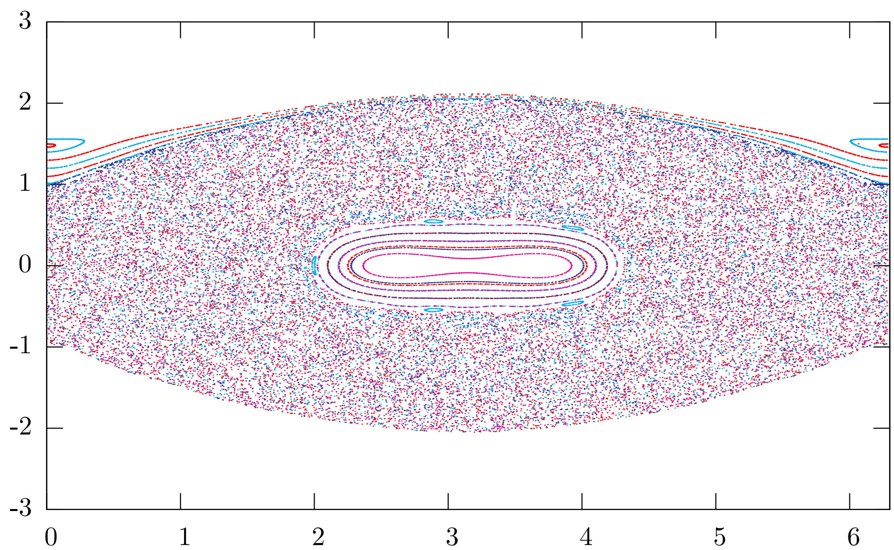


Figure 9: $A_x = 1,\ A_y = 1,\ B = 0.5,\ E = 0.75$

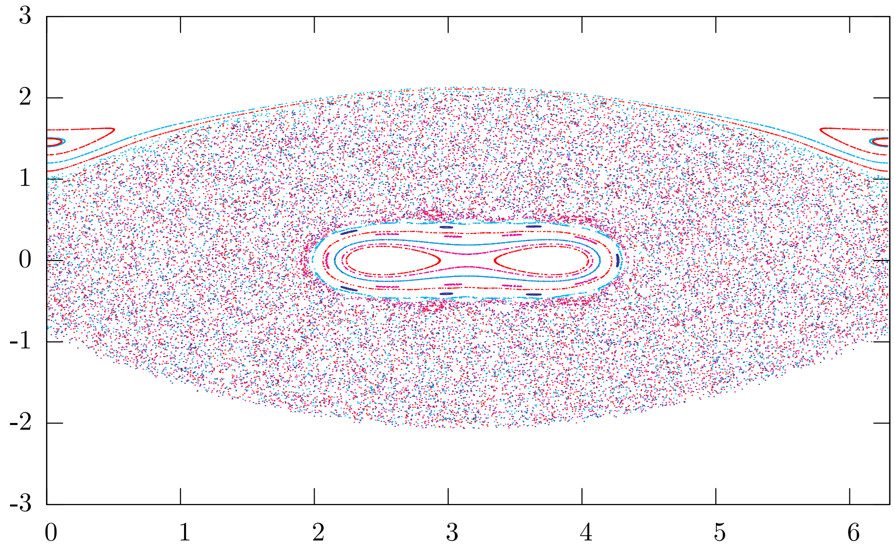


Figure 10: $A_x = 1,\ A_y = 1,\ B = 0.5,\ E = 0.80$

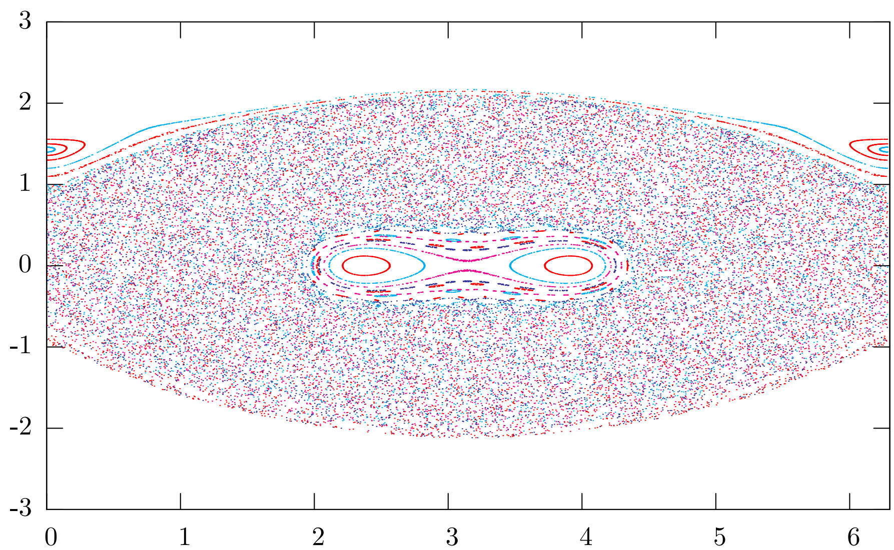


Figure 11: $A_x = 1,\ A_y = 1,\ B = 0.5,\ E = 0.85$

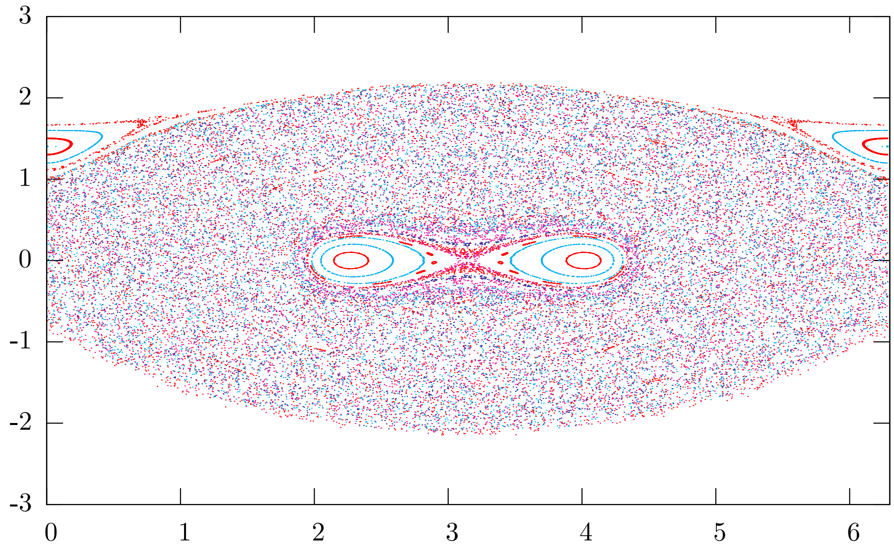


Figure 12: $A_x = 1$, $A_y = 1$, $B = 0.5$, $E = 0.90$

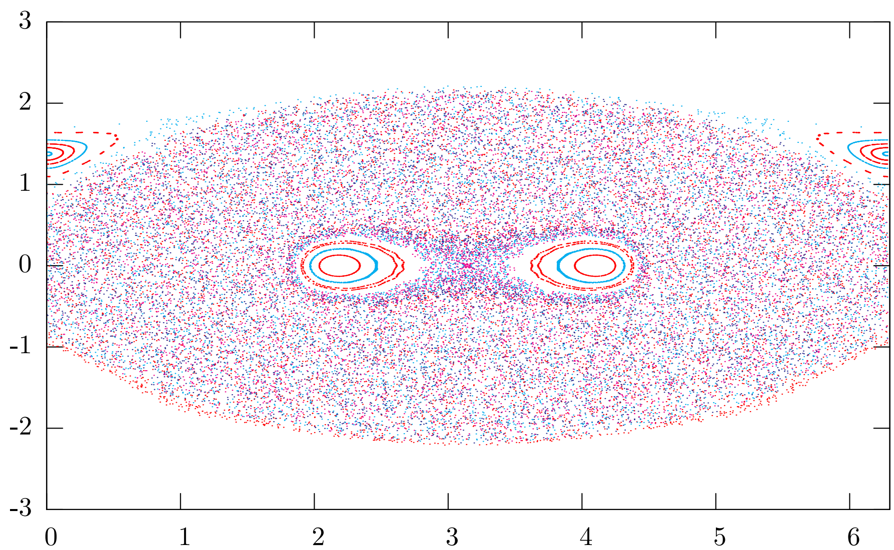


Figure 13: $A_x = 1$, $A_y = 1$, $B = 0.5$, $E = 0.95$

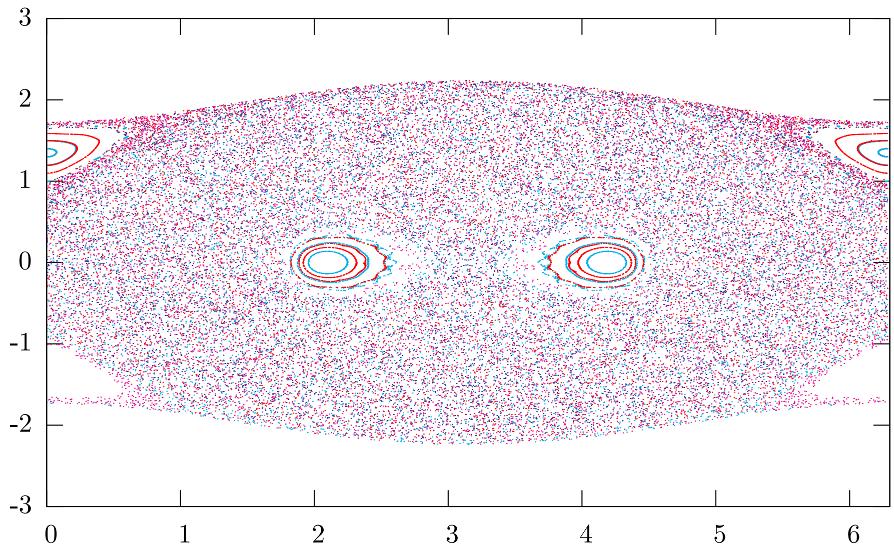


Figure 14: $A_x = 1,\ A_y = 1,\ B = 0.5,\ E = 1.00$

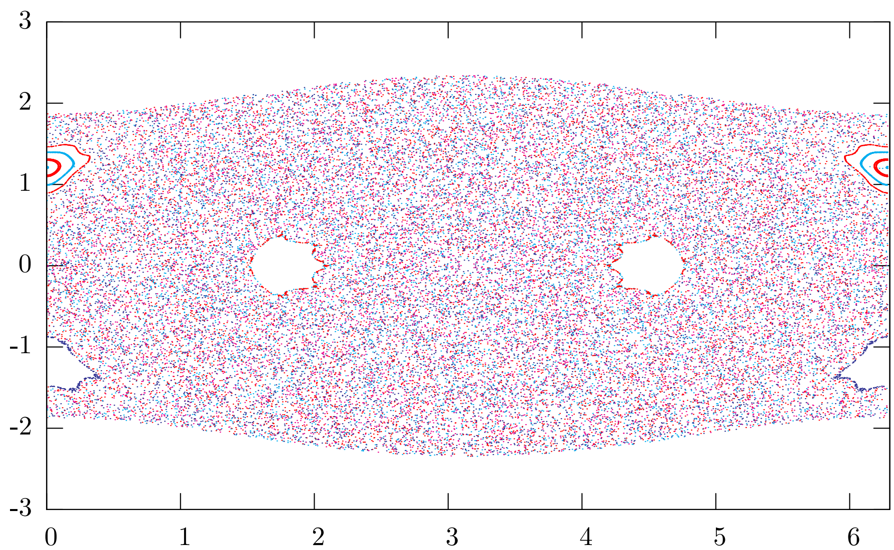


Figure 15: $A_x = 1,\ A_y = 1,\ B = 0.5,\ E = 1.25$

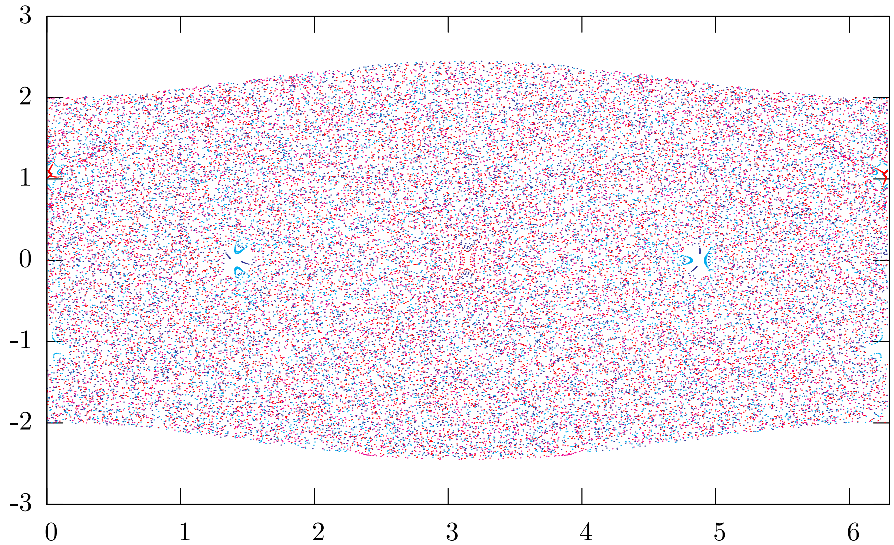


Figure 16: $A_x = 1,\ A_y = 1,\ B = 0.5,\ E = 1.50$

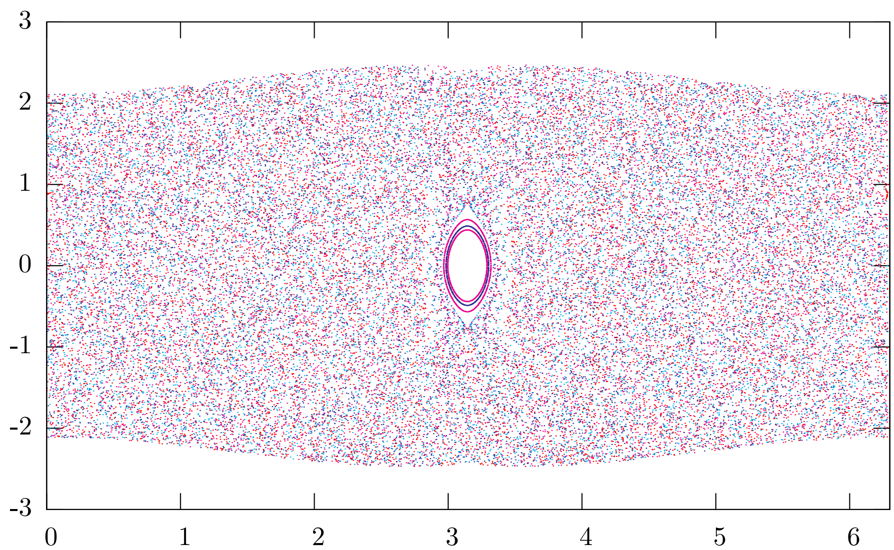


Figure 17: $A_x = 1,\ A_y = 1,\ B = 0.5,\ E = 1.75$

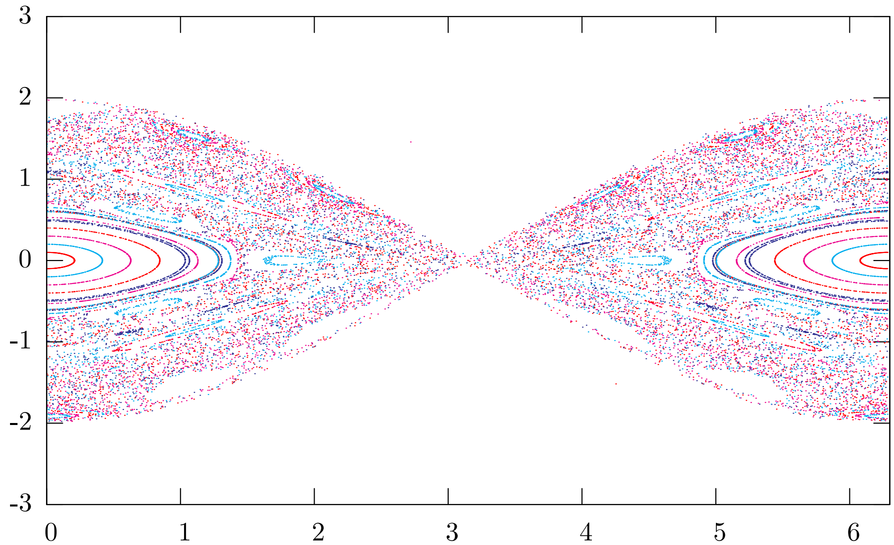


Figure 18: $A_x = 1,\ A_y = 1,\ B = 2,\ E = 0.00$

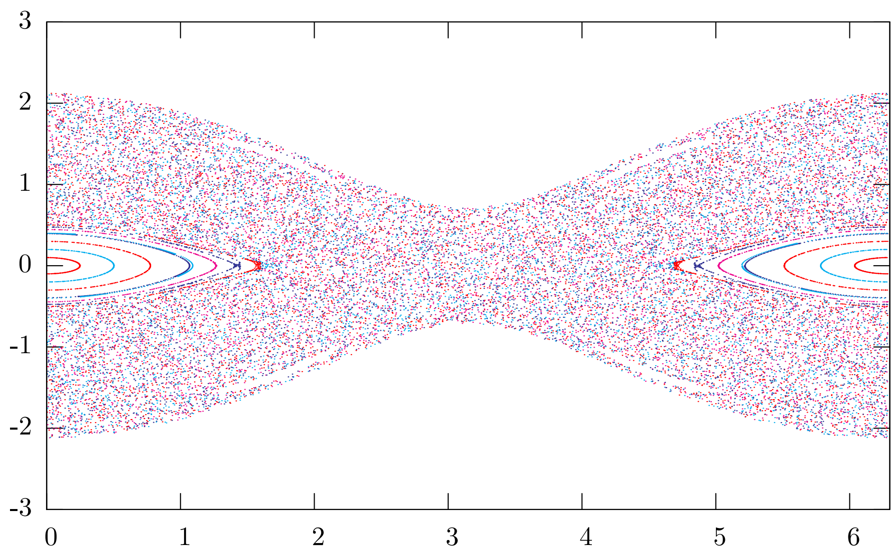


Figure 19: $A_x = 1,\ A_y = 1,\ B = 2,\ E = 0.25$

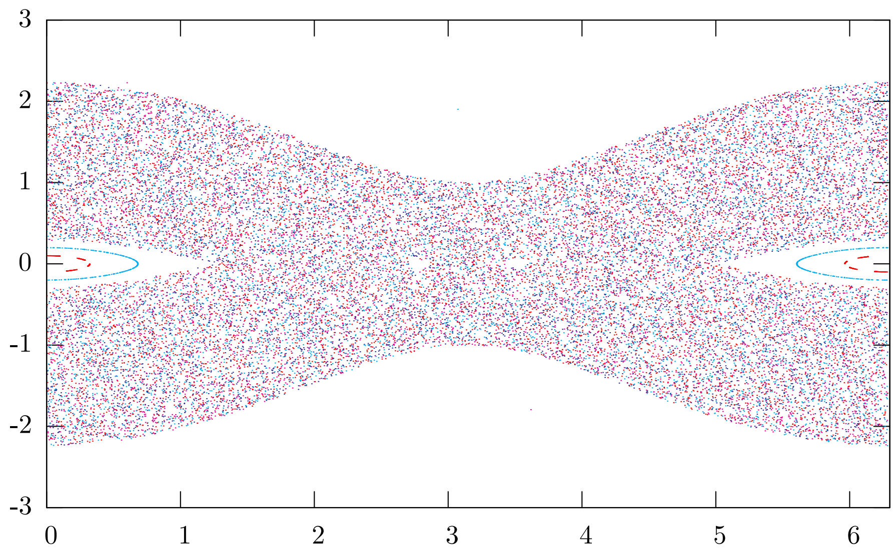


Figure 20: $A_x = 1,\ A_y = 1,\ B = 2,\ E = 0.50$

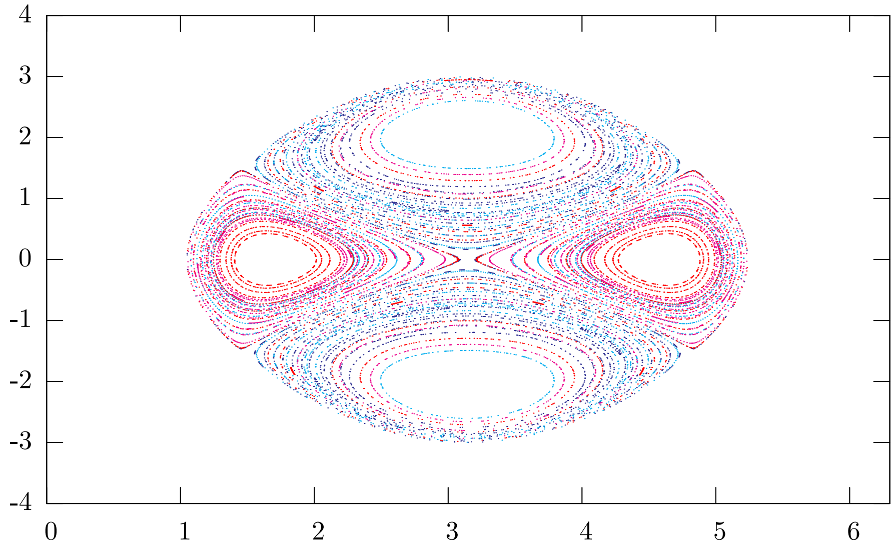


Figure 21: $A_x = 1,\ A_y = 1,\ B = -2,\ E = 0.50$

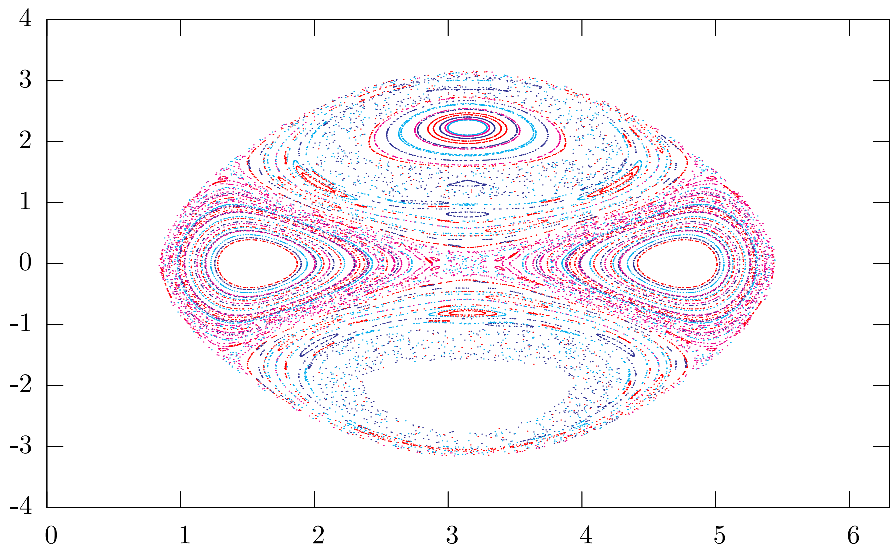
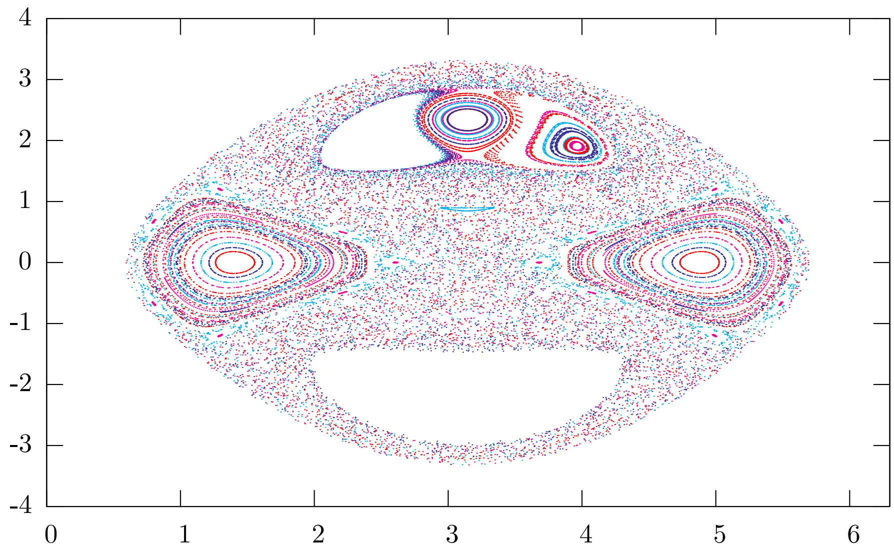


Figure 22: $A_x = 1,\ A_y = 1,\ B = -2,\ E = 1.00$



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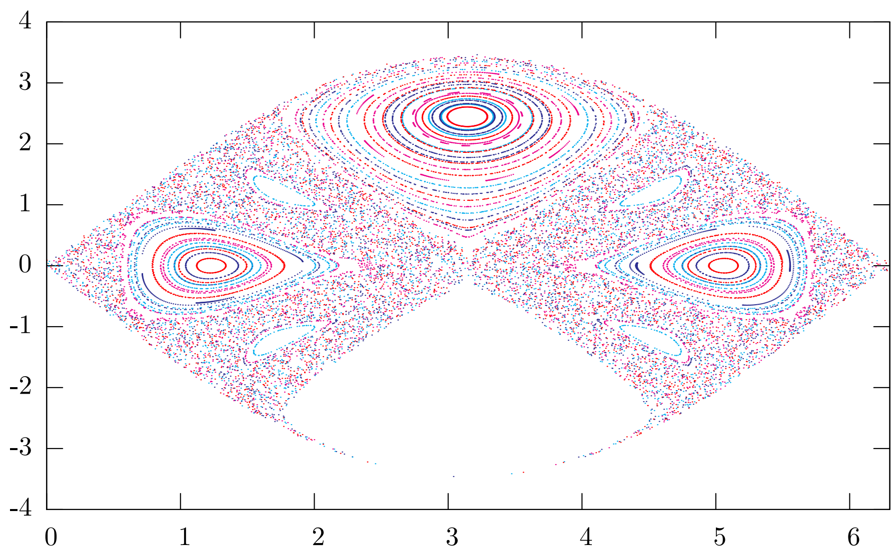

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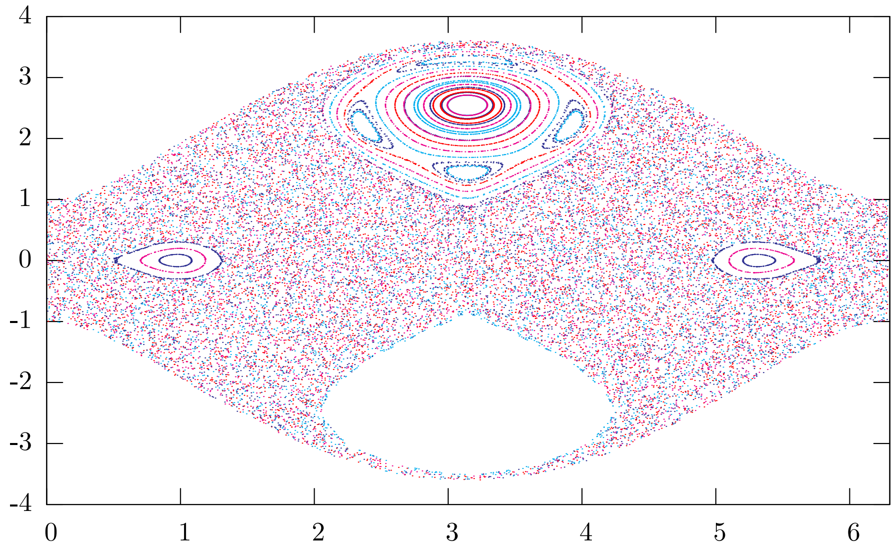

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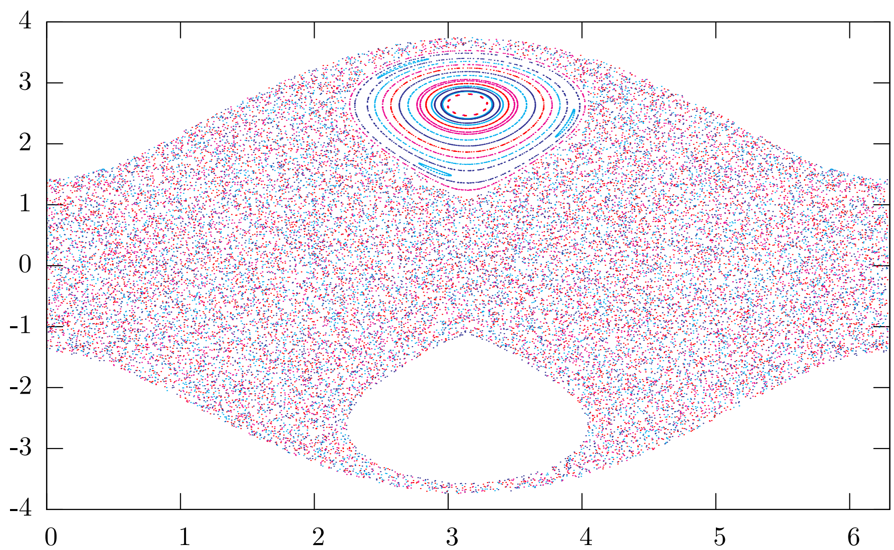

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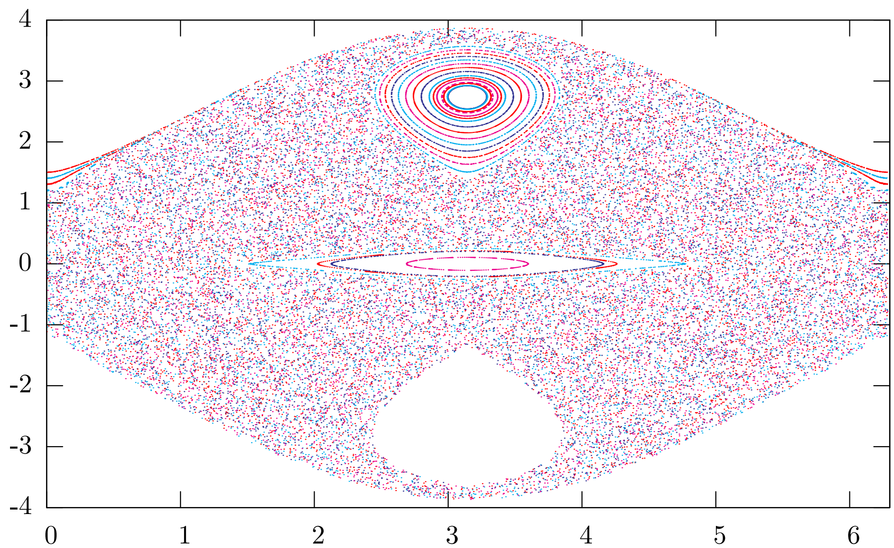

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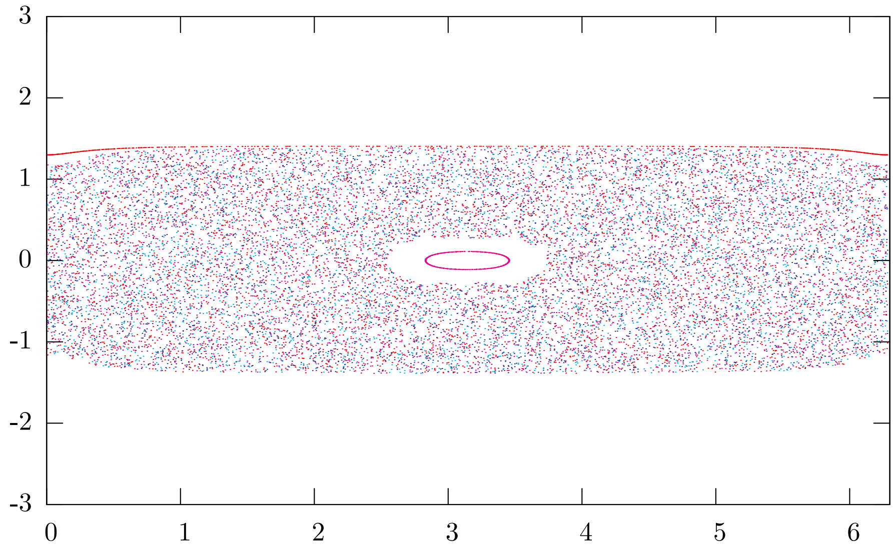
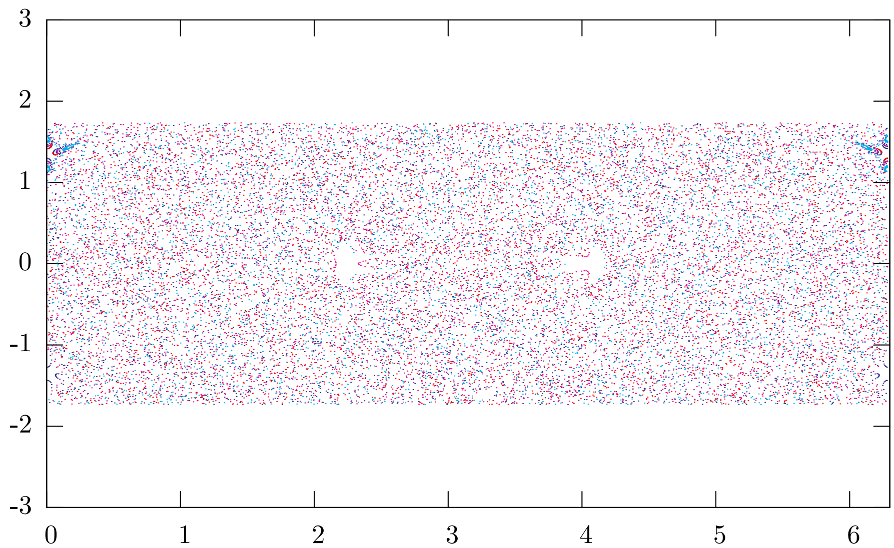


Figure 28: $A_x = 1,\ A_y = 1,\ B = 1,\ E = 0.00$



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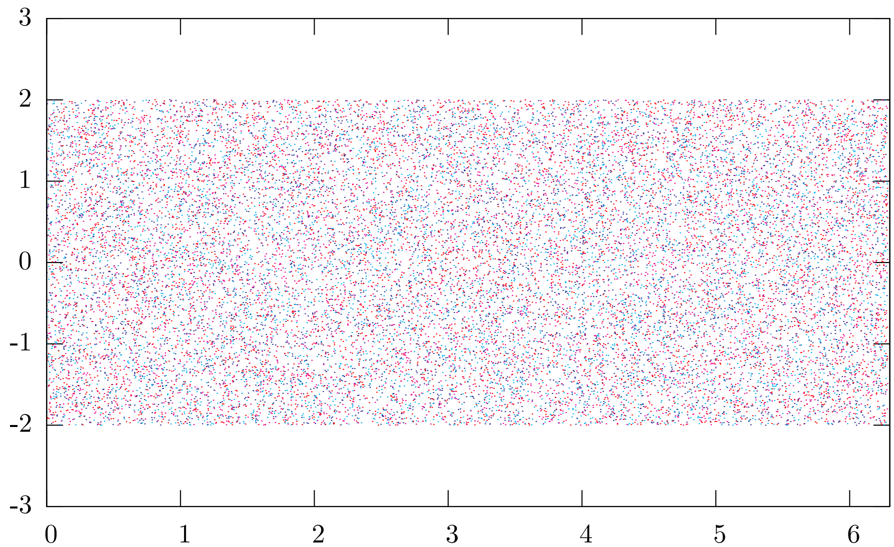

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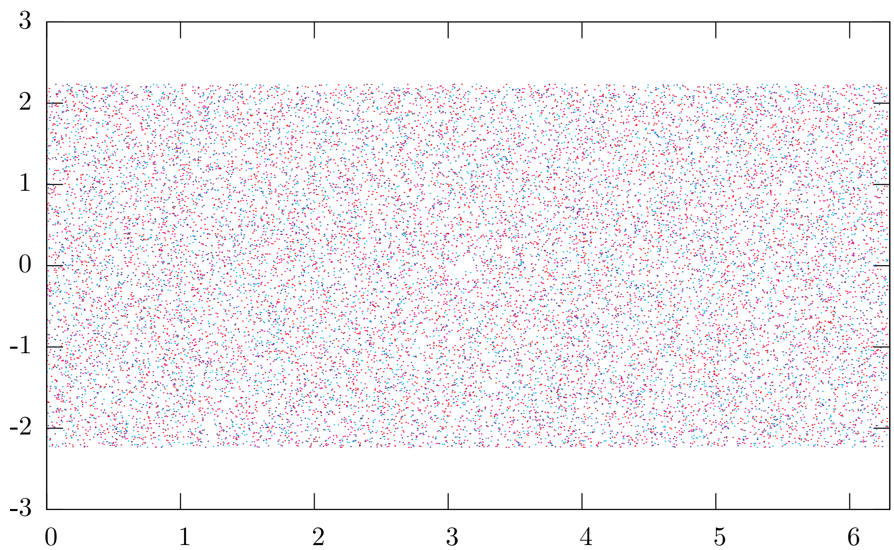

Figure 31: $A_x = 1,\ A_y = 1,\ B = 1,\ E = 1.50$

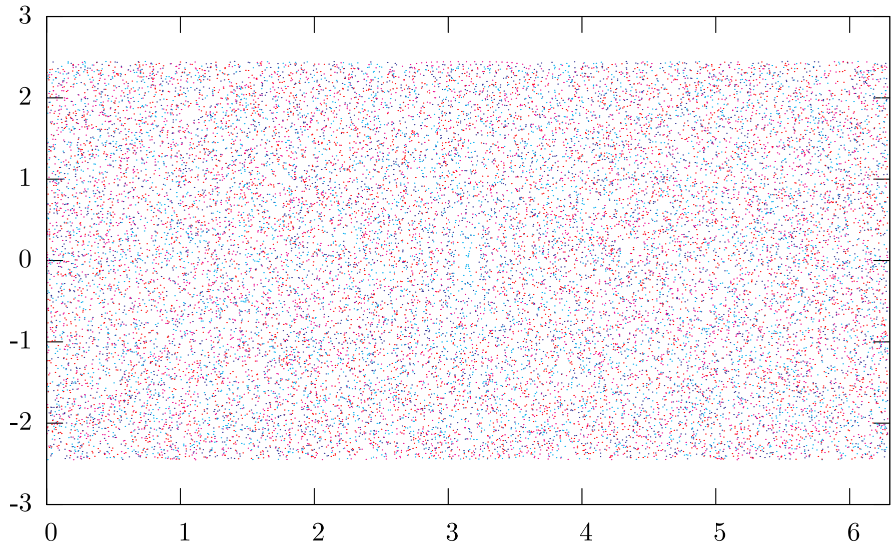

Figure 32: $A_x = 1,\ A_y = 1,\ B = 1,\ E = 2.00$

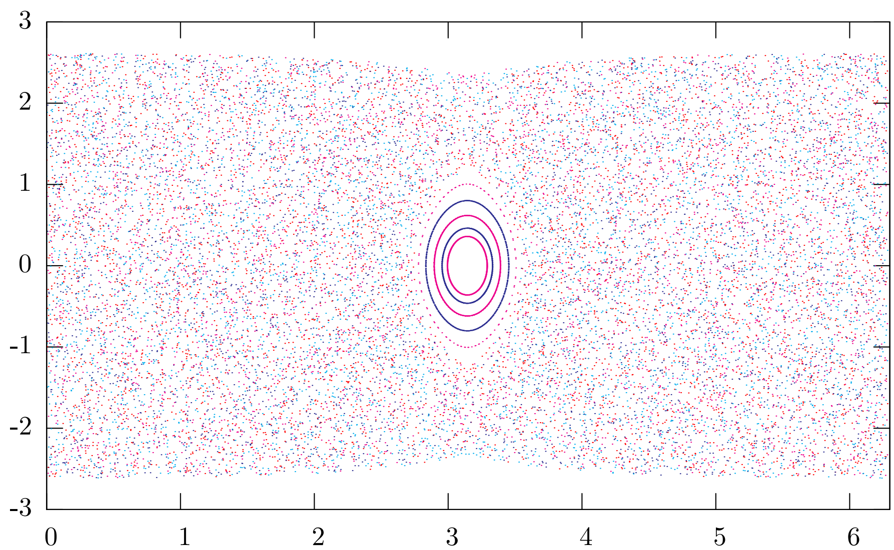

Figure 33: $A_x = 1,\ A_y = 1,\ B = 1,\ E = 2.50$