Localized Control of 1-Dimensional Perturbed Hydrogen Atom

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The method of Refs.[1–5] for localized control is implemented on 1-dimensional hydrogen atom perturbed by external field. A small control term added to the unperturbed Hamiltonian leads to barriers which confine phase space trajectories.

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I. INTRODUCTION

My project is an approach to a localized control of 1-dimensional hydrogen atom perturbed by a weak external field. Chaos control of dynamical systems has been an interesting, challenging and important topic in recent years. Most traditional control methods do change the properties of the original system although that is not desired. In this project, I applied a novel method [1–5] to 1-dimensional perturbed hydrogen atom to make localized control without significantly changing the properties of original system. I implement computation and obtain a small control term which was added to the uncontrolled Hamiltonian in order to build barriers confining trajectories in phase space.

II. HAMILTONIAN OF 1-DIMENSIONAL HYDROGEN ATOM

Simultaneously choosing the electron mass, Coulomb's constant and the electron charge the value unity, we have the Hamiltonian of 1-dimensional hydrogen atom with a weak perturbed external field

$$H(p,x,t) = \frac{p^2}{2} - \frac{1}{x} + \lambda x \cos \omega t,$$

where λ could be considered constant related to the amplitude of external field. My goal is to implement localized control method of Refs.[1–5] to this system. A barrier should be built to confine trajectories in phase space such that the system becomes more regular, but keeping the properties of chaotic structure unaltered.

III. LOCALIZED CHAOS CONTROL

A novel localized control method was proposed in Refs.[1–5] along with detailed mathematical proofs and derivations. Here I briefly review it, and in the following sections apply this method to 1-dimensional perturbed hydrogen atom problem.

Suppose the perturbed Hamiltonian can be written in action-angle variables $I(A,\widetilde{\theta})$ with L degrees of freedom

$$H(A,\widetilde{\theta}) = \omega \cdot A + V(A,\widetilde{\theta}) \tag{1}$$

where $(A,\widetilde{\theta}) \in \mathbf{R}^L \times \mathbf{T}^L$, and ω is a non-resonant vector of $\mathbf{R}^L$. The $V(A,\widetilde{\theta})$ may be expanded and written as

$$V(A,\widetilde{\theta}) = \varepsilon v(\widetilde{\theta}) + \varepsilon w(\widetilde{\theta}) \cdot A + Q(A,\widetilde{\theta}), \tag{2}$$

where the first term of right hand side is a constant part, the second term is a linear part in actions of order ε, and Q stands for the terms with order of actions higher than 1. Here we assume that the unperturbed Hamiltonian has an invariant torus with frequency vector ω at $A = 0$. This assumption is reasonable since we can easily do translation to achieve it, if originally $A \neq 0$. Also note $V(A,\widetilde{\theta})$ is not original perturbation term but represents some terms in the form described in equation (2) above. Then the controlled Hamiltonian can be constructed as

$$H_c(A,\widetilde{\theta}) = \omega \cdot A + V(A,\widetilde{\theta}) + f(\widetilde{\theta})\Omega(A,\widetilde{\theta})$$

where Ω is a smooth characteristic function which could be chosen $\Omega = 1$ if we intend to apply control term $f(\widetilde{\theta})$ in all phase space. Somewhat surprising is that additional resonances introduced by control term do reduce chaos which is contrary to expectation of Chirikov's criterion [6] stating that more overlaps of resonant islands cause

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more chaos. The control term $f(\widetilde{\theta})$ depends only on angle variables and has the form

$$f(\widetilde{\theta}) = V(0,\widetilde{\theta}) - V(-\Gamma\partial_{\widetilde{\theta}}V(0,\widetilde{\theta}),\widetilde{\theta}) \tag{3}$$

where Γ is a linear operator defined as a pseudo-inverse of $\omega\cdot\partial_{\widetilde{\theta}}$. One choice of Γ acting on $V=\sum_k V_k e^{i\widetilde{\theta}\cdot k}$ is

$$\Gamma V = \sum_{\omega\cdot k\neq 0} \frac{V_k}{i\omega\cdot k} e^{i\widetilde{\theta}\cdot k} \tag{4}$$

The control term is supposed to be relatively small compared with perturbation term. As to a specific 1-dimensional perturbed hydrogen atom problem, a canonical transformation converting p, x variables into action-angle variables is necessary and after that more steps would be taken to make the perturbed Hamiltonian in the form of equation (1) and (2) so that control term formula (3) may be applied.

IV. IMPLEMENTATION, 1-DIMENSIONAL PERTURBED HYDROGEN ATOM

The Hamiltonian of 1-dimensional hydrogen atom in a weak perturbed external field is

$$H(p,x,t) = \frac{p^2}{2} - \frac{1}{x} + \lambda x\cos\omega t \tag{5}$$

Note the unperturbed Hamiltonian is conservative and the action-angle variables (J,θ) are given by the famous transformation [7]

$$x = 2J^2\sin^2\varphi \qquad p = \frac{1}{J}\cot\varphi$$

with

$$\theta = 2\varphi - \sin 2\varphi$$

Then the Hamiltonian(5) becomes

$$H(J,\theta,t) = -\frac{1}{2J^2} + 2J^2\lambda\sin^2\varphi\cos\omega t \tag{6}$$

Now we take Fourier expansion to the 2nd term of right hand side of Hamiltonian (6), it turns out to be

$$H = -\frac{1}{2J^2} + 2J^2\lambda(\frac{a_0}{2} + \sum_{n=1}^{\infty} a_n\cos n\theta)cos\omega t \tag{7}$$

where

$$\begin{aligned} a_n &= \frac{1}{\pi}\int_{-\pi}^{\pi}\sin^2\varphi\cos n\theta d\theta \\ &= \frac{J_n(n) - J_{n-1}(n)}{n} \end{aligned} \tag{8}$$

where J_n is the Bessel function of the first kind. Equation (7) also leads to

$$\begin{aligned} H &= -\frac{1}{2J^2} + \lambda J^2(a_0\cos\omega t \\ &\quad + \sum_{n=1}^{\infty} a_n[\cos(n\theta+\omega t) + \cos(n\theta-\omega t)]) \end{aligned} \tag{9}$$

In order to apply localized control theory described above, I need to make more transformations on equation (9) so that the Hamiltonian will be in the form of equation (1) [8].

After shifting the action J such that the invariant torus is located at $J=0$ [8], we have

$$\begin{aligned} H &= -\frac{1}{2(J+\omega_0^{-\frac{1}{3}})^2} + \lambda(J+\omega_0^{-\frac{1}{3}})^2(a_0\cos\omega t \\ &\quad + \sum_{n=1}^{\infty} a_n[\cos(n\theta+\omega t) + \cos(n\theta-\omega t)]) \end{aligned} \tag{10}$$

where ω_0 is Kepler frequency. If the perturbation term in Hamiltonian (6) is taken off, the invariant tori are located at $J=\omega_0^{-1/3}$. Go ahead implementing Taylor expansion [8], we have

$$\begin{aligned} H &= -\frac{1}{2\omega_0^{-\frac{2}{3}}} + \omega_0 J - \frac{3\omega_0^{\frac{4}{3}}J^2}{2} + \sum_{k=3}^{\infty} C_k J^k \\ &\quad + \lambda(J^2 + 2\omega_0^{-\frac{1}{3}}J + \omega_0^{-\frac{2}{3}})(a_0\cos\omega t \\ &\quad + \sum_{n=1}^{\infty} a_n[\cos(n\theta+\omega t) + \cos(n\theta-\omega t)]) \end{aligned} \tag{11}$$

Since the first term of Hamiltonian is a constant, it doesn't matter to neglect it. Also, to make the Hamiltonian above time-independent, we add up an additional term E as the second angle variable which is canonically conjugate to time(Actually in Poincaré surface of section plotting, if we take $\omega=1$ then time can be considered time mod 2π due to the periodicity). Then it comes out the autonomous Hamiltonian

$$\begin{aligned} H &= E + \omega_0 J - \frac{3\omega_0^{\frac{4}{3}}J^2}{2} + \sum_{k=3}^{\infty} C_k J^k \\ &\quad + \lambda(J^2 + 2\omega_0^{-\frac{1}{3}}J + \omega_0^{-\frac{2}{3}})(a_0\cos\omega t \\ &\quad + \sum_{n=1}^{\infty} a_n[\cos(n\theta+\omega t) + \cos(n\theta-\omega t)]) \end{aligned} \tag{12}$$

It's reasonable here for me to neglect terms $\sum_{k=3}^{\infty} C_k J^k$ and $\lambda(J^2)$ since they are in the high order of λ and relatively small. Then we end up with the autonomous Hamiltonian

$$\begin{aligned} H &= E + \omega_0 J - \frac{3\omega_0^{\frac{4}{3}}J^2}{2} + \lambda(2\omega_0^{-\frac{1}{3}}J + \omega_0^{-\frac{2}{3}})(a_0\cos\omega t \\ &\quad + \sum_{n=1}^{\infty} a_n[\cos(n\theta+\omega t) + \cos(n\theta-\omega t)]) \end{aligned} \tag{13}$$

where the frequency vector, the action variables and the angle variables are $\omega = (\omega_0, 1)$, $A = (J, E)$ and $\widetilde{\theta} = (\theta, t)$ respectively. Correspondingly,

$$V = -\frac{3\omega_0^{\frac{4}{3}} J^2}{2} + \lambda(2\omega_0^{-\frac{1}{3}} J + \omega_0^{-\frac{2}{3}})(a_0 \cos\omega t + \sum_{n=1}^{\infty} a_n[\cos(n\theta + \omega t) + \cos(n\theta - \omega t)]) \quad (14)$$

and

$$V(0, \theta, t) = \lambda\omega_0^{-\frac{2}{3}}(a_0 \cos\omega t + \sum_{n=1}^{\infty} a_n[\cos(n\theta + \omega t) + \cos(n\theta - \omega t)]) \quad (15)$$

After plugging equation (14) (15) into equation (3) and implementing the operation described by equation (4), we eventually obtain the localized control term

$$f(\widetilde{\theta}) = \lambda^2 \frac{3}{2}(\sum_{n=1}^{\infty} n a_n[\frac{\cos(n\theta + \omega t)}{n\omega_0 + \omega} + \frac{\cos(n\theta - \omega t)}{n\omega_0 - \omega}])^2 + \lambda^2 2\omega_0^{-1}(\sum_{n=1}^{\infty} n a_n[\frac{\cos(n\theta + \omega t)}{n\omega_0 + \omega} + \frac{\cos(n\theta - \omega t)}{n\omega_0 - \omega}])(a_0 \cos\omega t + \sum_{n=1}^{\infty} a_n[\cos(n\theta + \omega t) + \cos(n\theta - \omega t)]) \quad (16)$$

which could also be written as

$$f(\widetilde{\theta}) = \lambda^2 \frac{3}{2}(\sum_{n=1}^{\infty} n a_n[\frac{2n\omega_0 \cos n\theta \cos\omega t + 2\omega \sin n\theta \sin\omega t}{n^2\omega_0^2 - \omega^2}])^2 + \lambda^2 2\omega_0^{-1}(\sum_{n=1}^{\infty} n a_n[\frac{2n\omega_0 \cos n\theta \cos\omega t + 2\omega \sin n\theta \sin\omega t}{n^2\omega_0^2 - \omega^2}])(a_0 + 2\sum_{n=1}^{\infty} a_n \cos n\theta) \cos\omega t \quad (17)$$

It's obvious to notice that the location of constructed barrier depends on the choice of Kepler frequency ω_0. Without loss of generality, we take $\omega = 1$ to draw figures in this paper. The theoretical barrier curve is given by

$$J = \omega_0^{-\frac{1}{3}} - \lambda\omega_0^{-\frac{2}{3}} \sum_{n=1}^{\infty} \frac{2n^2 a_n \omega_0 \cos n\theta}{n^2\omega_0^2 - \omega^2} \quad (18)$$

The first term of right hand side in equation (18) comes from unperturbed Hamiltonian and the second term is determined by linear operation $-\Gamma\partial_{\widetilde{\theta}} V(0, \widetilde{\theta})$ in equation (3). Figure 1 shows Poincaré section of Hamiltonian (7) without control. Figure 2 shows Poincaré section of Hamiltonian (7) with full localized control term (17). In Figure 2, those trajectories launched below the constructed barrier $J \simeq 1.51$ are perfectly confined and never go to the upper region. Figure 3 and figure 4 respectively show uncontrolled and controlled trajectories only launched below the ω_0 dependent barrier $J \simeq 1.51$ for clearer comparison. Figure 5 and figure 6 respectively show uncontrolled and controlled trajectories launched below the barrier $J \simeq 1.65$ for clearer comparison.

V. SIMPLIFICATION OF LOCALIZED CONTROL TERM

However, localized control term (17) is still far away from what we want. We are expecting a control term in the form as simple as the applied weak external field. Therefore, more steps should be taken to simplify control term (17) although as a trade-off we may have an imperfect but acceptable control term eventually. The control term (17) consists of two terms. By plotting Poincaré sections we have verified that the first term is dominant in chaos control. Then the control term is now in the form

$$f(\widetilde{\theta}) = \lambda^2 \frac{3}{2}(\sum_{n=1}^{\infty} n a_n [\frac{2n\omega_0 \cos n\theta \cos\omega t + 2\omega \sin n\theta \sin\omega t}{n^2\omega_0^2 - \omega^2}])^2 \quad (19)$$

Figure 7 and figure 8 show Poincaré sections of Hamiltonian (7) with dominant control term (19).

However, control term (19) is still not good enough. An infinite form like equation (19) might be more understandable theoretically but less experimentally. Intuitively we can expect an approximate control term as simple as the perturbation term.

Let's start from the control term (19) which could be written in the form

$$f(\widetilde{\theta}) = \lambda^2 \frac{3}{2}(\sum_{n=1}^{\infty} n a_n[\frac{\cos(n\theta + \omega t)}{n\omega_0 + \omega} + \frac{\cos(n\theta - \omega t)}{n\omega_0 - \omega}])^2 \quad (20)$$

and also take the assumed simplified control term

$$f_c(p, x, t) = Fx \cos\omega_c t \quad (21)$$

which could be written in the form of action-angle variables

$$f_c(J, \theta, t) = FJ^2(a_0 \cos\omega_c t + \sum_{n=1}^{\infty} a_n[\cos(n\theta + \omega_c t) + \cos(n\theta - \omega_c t)]) \quad (22)$$

where F is a very small number which needs to be determined and ω_c could be chosen related to the frequency of the perturbation field ω. After shifting the action J such that the torus is located at $J=0$, we have

$$\begin{aligned} f_c(J,\theta,t) &= F(J^2+2\omega_0^{-\frac{1}{3}}J+\omega_0^{-\frac{2}{3}})(a_0\cos\omega_c t \\ &\quad + \sum_{n=1}^{\infty} a_n[\cos(n\theta+\omega_c t)+\cos(n\theta-\omega_c t)]) \end{aligned} \tag{23}$$

By comparing equation (23) to equation (20) and choosing $\omega_c = 2\omega$, we can construct an approximate equation for F

$$F\omega_0^{-\frac{2}{3}}a_{2n+1} = \lambda^2 \frac{3}{2}\frac{n(n+1)a_n a_{n+1}}{(n\omega_0-\omega)((n+1)\omega_0-\omega)} \tag{24}$$

with

$$\omega_0 \in [\frac{\omega}{n+1},\frac{\omega}{n}]$$

Consequently we have

$$F = \frac{3}{2}\lambda^2\omega_0^{\frac{2}{3}}\frac{n(n+1)a_n a_{n+1}}{a_{2n+1}(n\omega_0-\omega)((n+1)\omega_0-\omega)} \tag{25}$$

with

$$\omega_0 \in [\frac{\omega}{n+1},\frac{\omega}{n}]$$

Plugging equation (25) and $\omega_c = 2\omega$ into equation (21), we obtain the simplified control term

$$f_c(p,x,t) = \frac{3}{2}\lambda^2\omega_0^{\frac{2}{3}}\frac{n(n+1)a_n a_{n+1}x\cos 2\omega t}{a_{2n+1}(n\omega_0-\omega)((n+1)\omega_0-\omega)} \tag{26}$$

which is in the form of weak microwave field. Figure 9 and figure 10 show Laminar plots of Hamiltonian with and without simplified control term (22) respectively. If a launched trajectory from a certain region exceeds the preset exit value after some iterations, then it is considered to have escaped from the system. Therefore bluer colors stand for the regions from which the trajectories are much easier to escape than redder color regions. We can notice the evident difference between figure 9 and figure 10 especially around the three resonant islands. The chaos is reduced to some extent by control term (22) although not perfectly since control term (22) has been highly simplified.

VI. FUTURE WORK

Simplified control term (22) is far away from full control term (17) as described above. With full control term (17), one can expect a Laminar plot almost composed of two uniform colors, deep blue above and deep red below the barrier curve. Therefore the work to keep searching for better simplified control term is ahead.

Another piece of work one might be interested in is to apply the localized control theory to 2-dimensional hydrogen atom problem. The Hamiltonian of 2-dimensional hydrogen atom with external field in atomic units is

$$H = \frac{p_x^2+p_y^2}{2} - \frac{1}{\sqrt{x^2+y^2}} + \lambda x\cos\omega t \tag{27}$$

The Hamiltonian above can be expressed in terms of action angle variables $(I_n, I_l, \theta_n, \theta_l)$ [9]

$$H = -\frac{1}{2}I_n^{-2} + \lambda(\xi\cos\theta_l - \eta\sin\theta_l)\cos\omega t \tag{28}$$

where

$$\xi = -\frac{3I_n^2\varepsilon}{2} + 2I_n^2\sum_{s=1}^{\infty}(\frac{1}{s}J_s'(s\varepsilon)\cos s\theta_n)$$

$$\eta = 2I_n^2(\varepsilon^{-2}-1)^{\frac{1}{2}}\sum_{s=1}^{\infty}(\frac{1}{s}J_s(s\varepsilon)\sin s\theta_n)$$

$$\varepsilon^2 = 1-\frac{I_l^2}{I_n^2}$$

Carrying out the same processes as 1-dimensional problem, we will be still able to apply localized control theory to obtain desired control term for 2-dimensional problem although the computation is much more complicated due to the presence of parameter ε and one more involved action angle variable set.

In addition to those work above, I'd like to concentrate on ionization of hydrogen Rydberg atoms in external fields which is a relatively big topic.

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APPENDIX A: PROJECT PLAN

Schedule of which part I intend to deliver by which date:

1. **Mon May 2:** Polish the project to high shine. Project deadline

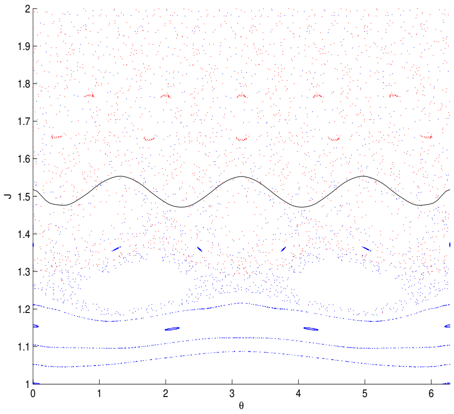

Fig. 1: Poincaré surface of section of Hamiltonian (7) with $\lambda = 0.01$, $\omega = 1$ and n up to 20.

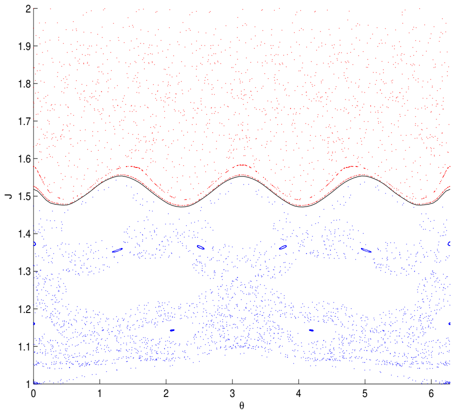

Fig. 2: Poincaré surface of section of Hamiltonian (7) with localized control term (17) with $\lambda = 0.01$, $\omega_0 = 1.51^{-3}$, $\omega = 1$ and n up to 20.

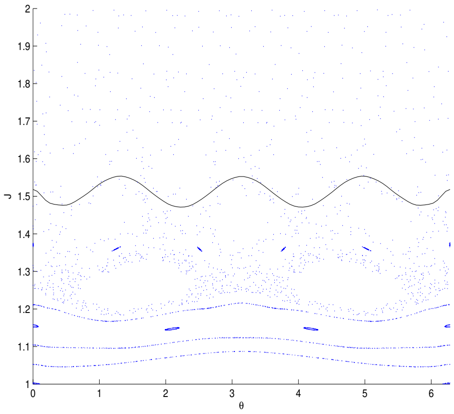

Fig. 3: Poincaré surface of section of Hamiltonian (7) launched below constructed barrier with $\lambda = 0.01$, $\omega = 1$ and n up to 20.

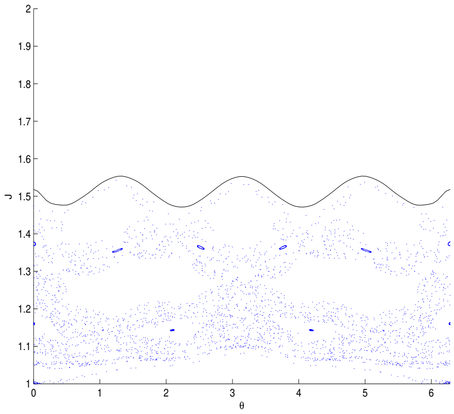

Fig. 4: Poincaré surface of section of Hamiltonian (7) launched below constructed barrier with localized control term (17) with $\lambda = 0.01$, $\omega_0 = 1.51^{-3}$, $\omega = 1$ and n up to 20.

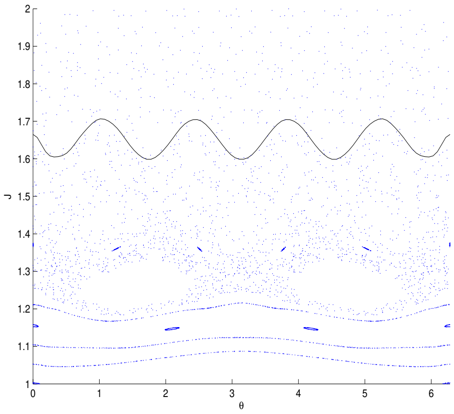

Fig. 5: Poincaré surface of section of Hamiltonian (7) launched below constructed barrier with $\lambda = 0.01$, $\omega = 1$ and n up to 20.

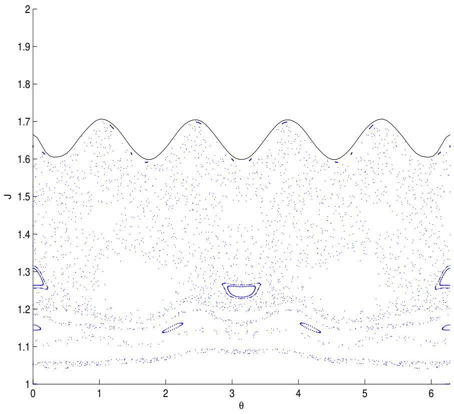

Fig. 6: Poincaré surface of section of Hamiltonian (7) launched below constructed barrier with localized control term (17) with $\lambda = 0.01$, $\omega_0 = 1.65^{-3}$, $\omega = 1$ and n up to 20.

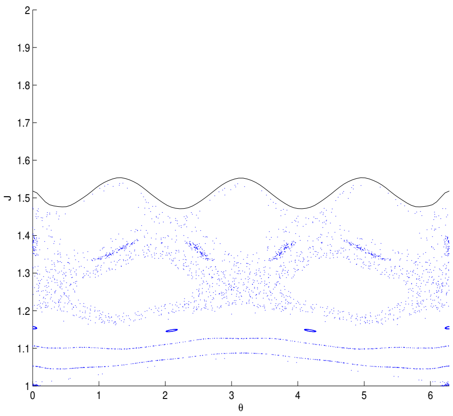

Fig. 7: Poincaré surface of section of Hamiltonian (7) launched below constructed barrier with localized control term (19) with $\lambda = 0.01$, $\omega_0 = 1.51^{-3}$, $\omega = 1$ and n up to 20.

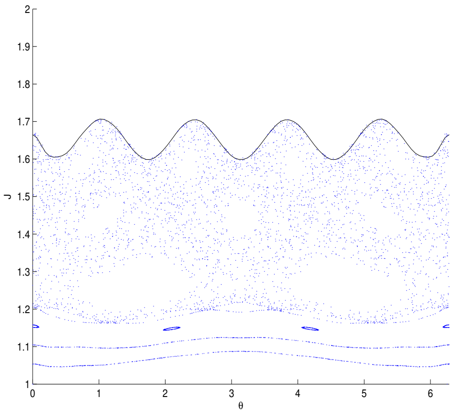

Fig. 8: Poincaré surface of section of Hamiltonian (7) launched below constructed barrier with localized control term (19) with $\lambda = 0.01$, $\omega_0 = 1.65^{-3}$, $\omega = 1$ and n up to 20.

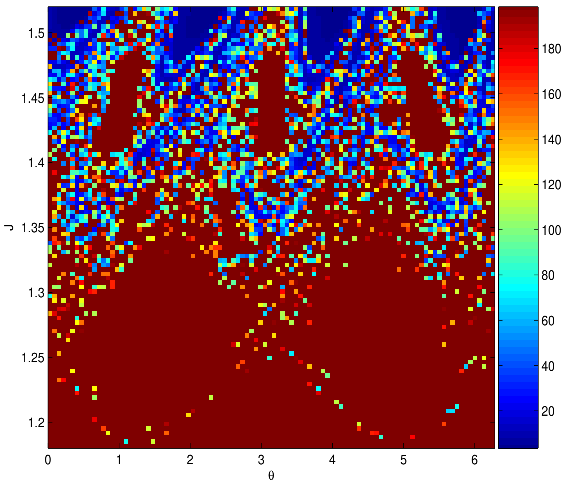

Fig. 9: Laminar plot of Hamiltonian (7) with $\lambda = 0.01$, $\omega_0 = 1.51^{-3}$, $\omega = 1$, n up to 20, exit value= 1.58 and maximal iteration= 200.

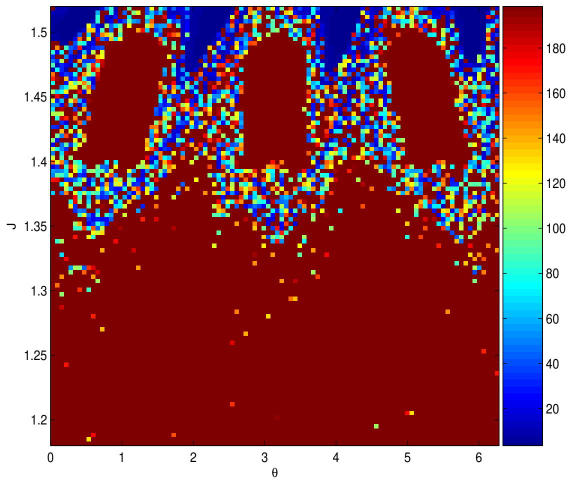

Fig. 10: Laminar plot of Hamiltonian (7) plus simplified control term (22) with $\lambda = 0.01$, $\omega_0 = 1.51^{-3}$, $\omega = 1$, n up to 20, exit value= 1.58 and maximal iteration= 200.