

Identification of multidimensional semiclassical tunneling paths

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Introduction

In the dynamical systems approach, the theory of turbulence for a given system, with given boundary conditions, is given by (a) the geometry of the state space and (b) the associated natural measure, that is, the likelihood that asymptotic dynamics visits a given state space region. We pursue this program in context of the Kuramoto-Sivashinsky (KS) equation, one of the simplest physically interesting spatially extended nonlinear systems.

Dynamical state space representation of a PDE is ∞ -dimensional, but the KS flow is strongly contracting and its non-wondering set, and, within it, the set of invariant solutions investigated here, is embedded into a finite-dimensional inertial manifold [?] in a non-trivial, nonlinear way. ‘Geometry’ in the title of this paper refers to our attempt to systematically triangulate this set in terms of dynamically invariant solutions (equilibria, periodic orbits, . . .) and their unstable manifolds, in a PDE representation and numerical simulation algorithm independent way. The goal is to describe a given ‘turbulent’ flow quantitatively, not model it qualitatively by a low-dimensional model.

In previous work, the state space geometry and the natural measure for this system have been studied [?, ?, ?] in terms of unstable periodic solutions restricted to the antisymmetric subspace of the KS dynamics. The focus in this paper is on the role continuous symmetries play in spatiotemporal dynamics. The notion of exact periodicity in time is replaced by the notion of relative spatiotemporal periodicity, and relative equilibria and relative periodic orbits here play the role the equilibria and periodic orbits played in the earlier studies.

Building upon the pioneering work of refs. [?, ?], we undertake here a study of the Kuramoto-Sivashinsky dynamics for a specific system size $L = 22$, sufficiently large to exhibit many of the features typical of ‘turbulent’ dynamics observed in large KS systems, but small enough to lend itself to a detailed exploration of the equilibria and relative equilibria, their stable/unstable manifolds, determination of a large number of relative periodic orbits, and a preliminary exploration of the relation between the observed spatiotemporal ‘turbulent’ patterns and the relative periodic orbits.

Kuramoto-Sivashinsky equation

The Kuramoto-Sivashinsky [henceforth KS] system [?, ?], which arises in the description of stability of flame fronts, reaction-diffusion systems and many other physical settings [?], is one of the simplest nonlinear PDEs that exhibit spatiotemporally chaotic behavior. In the formulation adopted here, the time evolution of the ‘flame front velocity’ $u = u(x, t)$ on a periodic domain $u(x, t) = u(x + L, t)$ is given by

$$u_t = F(u) = -\frac{1}{2}(u^2)_x - u_{xx} - u_{xxx}, \quad x \in [-L/2, L/2]. \quad (1)$$

Here $t \geq 0$ is the time, and x is the spatial coordinate. The subscripts x and t denote partial derivatives with respect to x and t . In what follows we shall state results of all calculations either in units of the ‘dimensionless system size’ \tilde{L} , or the system size $L = 2\pi\tilde{L}$. Figure ?? presents a typical ‘turbulent’ evolution for KS. All numerical results presented in this paper are for the system size $\tilde{L} = 22/2\pi = 3.5014 \dots$

Symmetries of Kuramoto-Sivashinsky equation

G , the group of actions $g \in G$ on a state space (reflections, translations, *etc.*) is a symmetry of the KS flow (1) if $g u_t = F(gu)$. The KS equation is time translationally invariant, and space translationally invariant on a periodic domain under the 1-parameter group of $O(2) : \{\tau_{\ell/L}, R\}$. If $u(x, t)$ is a solution, then

$$\tau_{\ell/L} u(x, t) = u(x + \ell, t) \quad (2)$$

is an equivalent solution for any shift $-L/2 < \ell \leq L/2$, as is the reflection (‘parity’ or ‘inversion’)

$$R u(x) = -u(-x). \quad (3)$$

Equilibria and relative equilibria

Equilibria (or the steady solutions) are the fixed profile time-invariant solutions,

$$u(x, t) = u_q(x). \quad (4)$$

Due to the translational symmetry, the KS system also allows for relative equilibria (traveling waves, rotating waves), characterized by a fixed profile $u_q(x)$ moving with constant speed c , that is

$$u(x, t) = u_q(x - ct). \quad (5)$$

Here suffix $_q$ labels a particular invariant solution. Because of the reflection symmetry (3), the relative equilibria come in counter-traveling pairs $u_q(x - ct)$, $-u_q(-x + ct)$.

Relative periodic orbits, symmetries and periodic orbits

A relative periodic orbit satisfies

$$g u(x, T_p) = u(x, 0), \quad (6)$$

where $g \in G$, with G a symmetry of the flow. Thus, the KS equation can have relative periodic orbits corresponding to

1. Invariance under $\tau_{\ell/L}$

$$\tau_{\ell_p/L} u(x, T_p) = u(x + \ell_p, T_p) = u(x, 0) = u_p(x). \quad (7)$$

2. Invariance under reflections

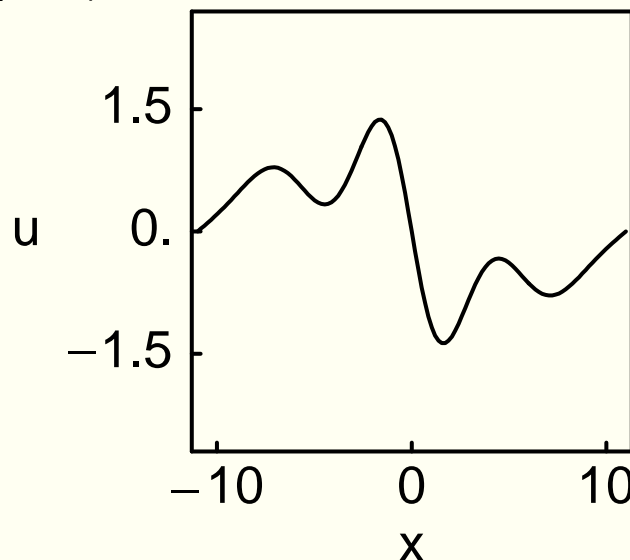
$$R u(x, T_p) = -u(-x, T_p) = u(x, 0) = u_p(x), \quad (8)$$

Such an orbit is pre-periodic to a periodic orbit with period $2T_p$.

Tunneling action

Freezing the transverse degrees of freedom to equilibrium reduces the normal form Hamiltonian to a one-dimensional tunneling Hamiltonian given as a power series in the tunneling action. This series can be inverted to obtain the action as a function of energy.

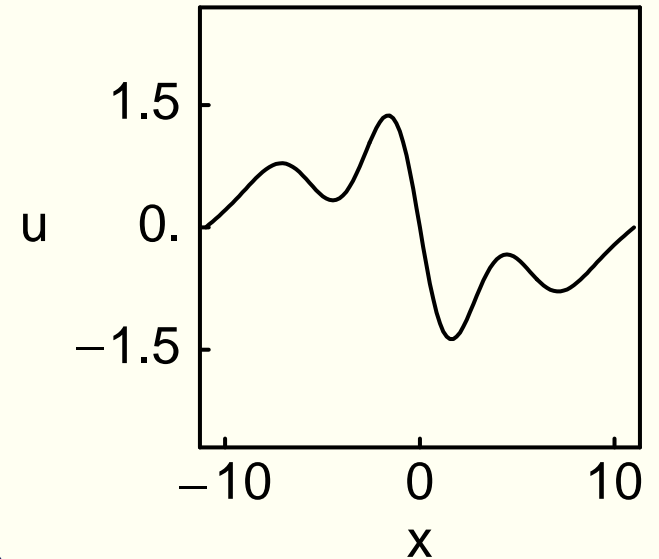
In practice, the power series for the action converges only very close to the saddle. By means of a Padé transform, however, useful values for the tunneling action can still be computed even far below the saddle point energy. It can then be observed how with increasing order the normal-form result converges to the action of the periodic tunneling orbit, whereas the action along the steepest-descent ‘reaction path’ is markedly larger and thus significantly underestimates the tunneling probability.



Transverse frequencies

In a similar manner, the frequencies of the transverse normal modes can be computed from the terms in the normal form Hamiltonian that are quadratic in the transverse coordinates.

In the figure, solid lines denote frequencies of the linearized motion around the periodic tunneling orbit. Dashed lines indicate frequencies obtained from a normal form calculation of order 4, 8, 12 or 16, respectively.



Effects of transverse modes

The optimal tunneling paths described above were calculated under the assumption that there is no excitation of the transverse degrees of freedom. In practice, however, the transverse modes will always be excited at least to their zero-point oscillations. The normal form approach to tunneling lends itself easily to an inclusion of transverse vibrations: It allows to construct a complete set of action coordinates that are conserved under the truncated dynamics. They can be set to arbitrary non-zero values if the corresponding nonlinear normal modes are excited. Then, as before, the normal form yields the energy as a power series in the tunneling action, which can be inverted to obtain the action as a function of energy.

References

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