Project description:

Quantization of strongly nonlinear field theories in terms of their unstable spatiotemporal periodic solutions

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1 Prelude

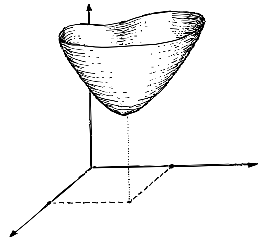
The project outlined in this proposal relies on concepts originating in several disparate disciplines: quantum field theory (path integrals), applied mathematics (fluid dynamics, amplitude equations), pure mathematics (spectral determinants, zeta functions) and atomic and nuclear physics (semi-classical quantization of helium, metastability of molecules and nuclei). In this preamble we will attempt to cover this background in a manner accessible to a non-specialist reviewer.

1.1 Challenge: semi-classical quantization of Quantum Field Theory

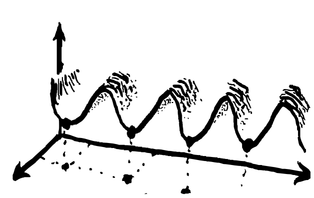
While very successful for quantum electrodynamics, the Feynman–diagrammatic perturbative expansions have been difficult to apply to strongly nonlinear field theories such as quantum chromodynamics. Nonlinear field theories appear to require radically different, non-perturbative approaches. In the 1970's a deeper appreciation of the connections between field theory and statistical mechanics led to path integral formulations such as the lattice QCD [1]. In lattice theories quantum fluctuations explore the full gauge group manifold, and classical dynamics of Yang-Mills fields plays no role.

We propose to re-examine here the path integral formulation and the role that the classical solutions play in quantization of strongly nonlinear fields. Out of necessity, this relies on a deeper understanding of dynamics of classical turbulence than what we currently possess, novel and powerful ideas will be needed to make progress on either front.

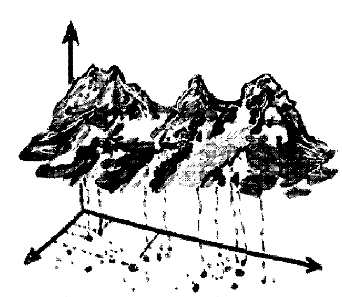
In the path integral formulation of a field theory the dominant contributions come from saddle-points, the classical solutions of equations of motion. Usually one imagines one dominant saddle point, the "vacuum":



one dominant extremum



an infinity of instanton saddles



a fractal set of saddles

But there might be other saddles. That field theories might have a rich repertoire of classical solutions became apparent with the discovery of instantons [2], analytic solutions of the classical $SU(2)$ Yang-Mills equations of motion, and the realization that the associated instanton vacuua receive contributions from ∞'s of saddles. What is not clear is whether these are the important classical saddles. Could it be that the strongly nonlinear theories are dominated by altogether different classical solutions?

The search for the classical solutions of nonlinear field theories such as the Yang-Mills and gravity has so far been neither very successful nor very systematic. The dynamics tends to be neglected, and understandably so, because the wealth of the classical solutions of nonlinear systems can be truly bewildering. If the classical behavior of these theories is anything like that of the field theories that describe the classical world — the hydrodynamics, the magneto-hydrodynamics – there should be very many solutions, with very few of the important ones analytical in form.

By late 1970's it was generally understood that even the simplest nonlinear systems exhibit chaos. Chaos is the norm also for generic Hamiltonian flows, and for path integrals that implies that instead of a few, or countably few saddles, classical solutions populate fractal sets of saddles. For the path-integral formulation of quantum mechanics such solutions were discovered and accounted for by Gutzwiller [3] in the early 1970's. In this framework the spectrum of the theory is computed from a fractal set, the set of its unstable classical periodic solutions.

We propose to formulate a semi-classical approximation to path integrals for strongly nonlinear field theories whose classical dynamics is turbulent in terms of an infinite hierarchy of unstable recurrent patterns. This will require a new type of Gutzwiller trace formula (described in sect. 2), and more powerful techniques for searching for unstable recurrent patterns (described in sect. 3).

1.2 Recurrent patterns

The inspiration for the "recurrent patterns program" comes from the way we perceive turbulence. Turbulent systems never settle down, but we can identify a snapshot as a "cloud", and an experimentalist can tell what the values of physical parameters in a turbulence experiment were after a glance at the digitized image of its output. How do we do it?

An answer was offered by E. Hopf [4]. In Hopf's vision turbulence explores a repertoire of distinguishable patterns; as we watch a "turbulent" system evolve, every so often we catch a glimpse of a familiar pattern:

$\Longrightarrow$ other swirls $\Longrightarrow$

For any finite spatial resolution, the system follows approximately for a finite time a pattern belonging to a finite alphabet of admissible patterns, and the long term dynamics can be thought of as a walk through the space of such patterns, just as chaotic dynamics with a low dimensional attractor can be thought of as a succession of nearly periodic (but unstable) motions. The periodic orbit theory (sketched here in sect. 2) provides the machinery that converts this intuitive picture into a precise calculational scheme. For extended systems the theory gives a description of the long time averages of observables in terms of short period recurrent spatio-temporal patterns.

So, if one is to develop a semiclassical field theory of systems that are classically chaotic or "turbulent," the first problem one faces is how to determine and classify the classical solutions of nonlinear field theories. Given how difficult the implementation of the periodic orbit theory can be already in finite dimensions, and the presence of features in the quantum field theory not captured by semiclassical expansions, its implementation in a full-fledged quantum field theory has for a long time seemed an overly ambitious project. *Recent exciting advances in the study of classical turbulence give us confidence that the steps toward this goal that we propose to investigate here are* *within the reach.*

1.3 1-d Kuramoto-Sivashinsky system

Field theories such as QCD, gravity or hydrodynamics have too many dimensions, symmetries, tensorial indices to be suited for exploratory forays into this forbidding terrain. We motivate the feasibility of the recurrent patterns program by one of the simplest and extensively studied spatially extended dynamical systems, the Kuramoto-Sivashinsky system [6] (see Holmes, Lumley and Berkooz [7] for a delightful introduction to the subject):

$$u_t = (u^2)_x - u_{xx} - \nu u_{xxxx} \tag{1}$$

which arises as an amplitude equation for interfacial instabilities such as flame fronts. Amplitude $u(x,t)$ has compact support, with $x \in [0, L]$ a periodic space coordinate. The $(u^2)_x$ term makes this a nonlinear system, t is the time, and ν is a "viscosity" damping parameter that irons out any sharp features. The solution $u(x,t) = u(x + L, t)$ is periodic on the $x \in [0, L]$ interval, so one usually expands $u(x,t)$ in a discrete spatial Fourier series

$$u(x,t) = i \sum_{k=-\infty}^{+\infty} a_k(t) e^{ikx} \,. \tag{2}$$

Restricting the considerations to the subspace of odd solutions $u(x,t) = -u(-x,t)$ for which a_k are real and substituting (2) into (1) yields the infinite ladder of evolution equations for the Fourier coefficients a_k:

$$\dot{a}_k = (k^2 - \nu k^4) a_k - k \sum_{m=-\infty}^{\infty} a_m a_{k-m} \,. \tag{3}$$

$u(x,t) = 0$ is a fixed point of (1), with the $k^2\nu < 1$ long wavelength modes of this fixed point linearly unstable, and the short wavelength modes stable.

On a finite size domain of length L the "Reynolds" parameter for the Kuramoto-Sivashinsky system is the dimensionless length $\tilde{L} = L/(2\pi\sqrt{\nu})$. For $\tilde{L} < 1$, $u(x,t) = 0$ is the globally attractive stable fixed point; as the system size $\tilde{L}$ is increased, the "flame front" becomes increasingly unstable and turbulent, the solutions go through a rich sequence of bifurcations, one quickly finds a myriad of unstable periodic solutions whose number grows exponentially with period.

In 1996 the PI's group was the first to propose that the periodic orbit theory be applied to spatio-temporal chaotic systems, using the Kuramoto-Sivashinsky system as a laboratory for exploring viability of the recurrent patterns program. The group [8] examined the dynamics of the periodic b.c., antisymmetric subspace, for values of the parameter $\tilde{L} \approx 2.889$, close to the onset of chaos, where a Galërkin truncation of (3) to 16 modes already yields accurate results. The main conceptual advance in this initial foray was the demonstration that the high-dimensional (16-64 dimensions) dynamics of this dissipative flow can be reduced to an approximately 1-dimensional Poincaré return map $s \to f(s)$, by choosing the unstable manifold of the shortest periodic orbit as the intrinsic curvilinear coordinate from which to measure near recurrences, see figure 1. This binary symbolic dynamics arising from this surprisingly simple return map made possible a systematic determination of *all* nearby unstable periodic orbits up to a given maximal period.

For the first time for any nonlinear PDE, some 1,000 prime cycles were determined numerically for various system sizes, with two typical ones plotted below in figure 4. What was novel about this work? First, dynamics on a strange attractor embedded in a high-dimensional space has been reduced to a 1-d map. Second, the solutions found provide both a *a qualitative description*, (in the sense that the Lorenz model captures qualitatively some of the bifurcations and chaos observed in full hydrodynamics) and a highly accurate *quantitative predictions* for a given PDE with given boundary conditions and a given "Reynolds" number.

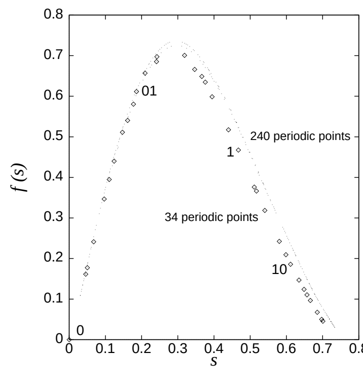


Figure 1: *The return map $s_{n+1} = f(s_n)$ constructed from periodic solutions of the Kuramoto-Sivashinsky equations (1), $\tilde{L} \approx 2.889$, with s the Euclidean distance measured along the unstable manifold of the fixed point $\overline{1}$. Periodic points $\overline{0}$ and $\overline{01}$ are also indicated. [8]*

In 1998 Zoldi and Greenside [9] investigated a considerably larger system, of size $\tilde{L} \approx 7.958$, spatially discretized, with fixed boundary conditions. Deploying a damped Newton method search on a supercomputer, initiated with 120,000 random initial conditions, they found 127 unstable periodic orbits. Their works illustrates some of the difficulties one faces in studying extended systems - blind periodic orbit searches do not necessarily find the orbits that belong to the asymptotic attractor. Most likely none of the unstable periodic orbits found in this study - all of them have as many as 3 to 8 unstable directions - participate in the asymptotic dynamics.

The essential limitation on the numerical studies undertaken in 1970's were the computational constraints: in truncation of high modes in the expansion (3), sufficiently many have to be retained to ensure the dynamics is accurately represented.

With the introduction of variational methods (described here in sect. 3) considerably *more turbulent regimes have become accessible, and will be investigated within the project proposed here.* We will focus on: (1) *elucidation of the phase-space flow topology and the symbolic dynamics for moderate finite sizes* $\tilde{L}$. (2) *search for the dominant short recurrent patterns for spatially infinite,* $\tilde{L} \to \infty$ *systems.*

1.4 Full Navier-Stokes: Plane Couette turbulence

While a good Galërkin truncation in the above Kuramoto-Sivashinsky system calculations requires of order of $10^1 - 10^3$ modes, the simplest Navier-Stokes calculation, the 3-d plane Couette flow, requires no less than $10^4 - 10^5$ modes, and any other classical field theory of interest will require orders of magnitude more than that. Is it possible to apply the methods that worked for the above 1-d model PDE to full fluid dynamics? Due to the sensitive dependence on initial conditions, and dramatic qualitative differences in dynamics at different system parameter values, already at moderate Rayleigh numbers the available nonlinear dynamics tools largely fail. Nevertheless, if one is interested in steady state turbulence at kitchen-faucet variety Reynolds numbers, the situation is not quite that scary. With the recent advances that we shall now describe, a way to a successful attack on the full 3-d Navier-Stokes problem is now within reach of the recurrent patterns program.

The reason is that in the long run a viscous flow, after the influence of the initial conditions has died down, converges to an "inertial manifold" $\mathcal{M}$ of a finite (but viscosity dependent and currently unknown) dimension. This finite dimensionality has been rigorously established by Foias and collaborators [10] in certain settings.

A very recent experiment [11] resolves the long standing puzzle of precise onset of turbulence in pipe flows by recasting the problem in clear dynamical systems terms: coexisting basins of attraction, with the laminar flow basin of stability in the sea of phase space shrinking as Re increases. The recently numerically discovered unstable nonlinear 3-d traveling wave solutions of the full Navier-Stokes [12] now make finding unstable recurrent patterns embedded in the strange attractor that supports sustained steady turbulence a high priority.

Computationally easier to deal with than the pipe flows, the plane shear flows are among the best studied hydrodynamic flows, both for the simplicity of the setting for fundamental studies of hydrodynamic turbulence, and for the engineering importance of the boundary layer turbulent drag. Easily visualized, they lend themselves to both colorful visualizations and colorful phenomenology, see Waleffe [13].

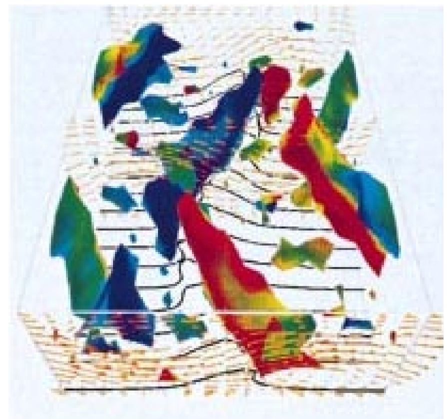


Figure 2: *A 3-d instantaneous snapshot of an unstable periodic solution embedded in the Couette turbulence [14]. Vectors and colors code velocities and vorticities.*

An example of what has already been attained, and what this project intends to push to a higher level, is the most impressive application of the recurrent patterns ideas to genuine fluid dynamics so far, by Kawahara and Kida [14]: the first demonstration of existence of an unstable recurrent pattern in a turbulent hydrodynamic flow. They have located an important unstable spatio-temporally periodic solution in a *15,422-dimensional* numerical discretization of the three-dimensional constrained plane Couette turbulence, with no-slip boundary conditions, at $Re = 400$. A 3-d snapshot of this solution at a given instant is given in figure 2.

Figure 3 illustrates why a single unstable periodic solution might already encode essential information about the turbulent flow. In the Couette flow energy is injected locally, through the drag exerted by the turbulent fluid on the two counter-moving plane walls, and consumed globally, by the viscous dissipation at small scales. Plotted horizontally is the energy input I, and vertically the dissipation D per unit time for a long-time simulation (green), for the periodic solution figure 2 (red), and for a short nearby segment of a typical trajectory (yellow). Were the dynamics laminar, the solution would be a stationary point at $(I, D) = (1, 1)$. The turbulent solution fluctuates by almost a factor of 2, with the mean turbulence-induced drag on the "airplane wing" substantially larger than what it would have been for a laminar flow, by a factor of nearly 3.

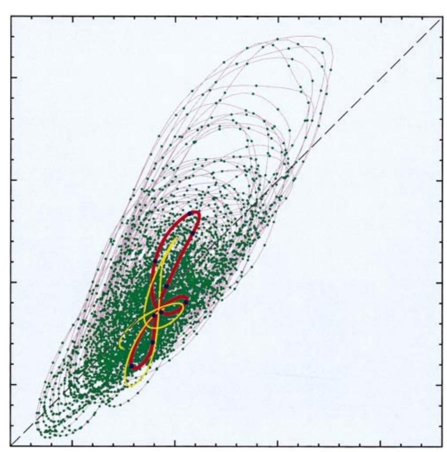


Figure 3: *Frictional drag vs. dissipation for the Couette turbulence. [14]*

Periodic orbit theory predicts the time averages and fluctuations of measurable quantities from their values computed on individual unstable periodic solutions. Accurate predictions require sets of the shortest periodic solutions. What is very encouraging about the Kawahara-Kida example is that already a *single unstable recurrent pattern* yields estimates of the mean dissipation D and mean velocity profiles across the Couette channel with a surprisingly high accuracy, presumably because it happens to explore the (infinite-dimensional) phase space region with the highest concentration of the natural measure.

At this point, the reviewer might wonder: in turbulence there is already vast knowledge about the various scaling laws dealing with energy, velocity, vorticity, and wavenumber statistics. Are the predictions of the proposed "recurrent patterns" theory consistent with the existing understanding? The recurrent patterns program does not address issues such as the Kolmogorov's 1941 homogeneous turbulence, with no coherent structures fixing the length scale; here all the action is in specific coherent structures. It does not seek universal scaling laws; spatio-temporally periodic solutions are specific to the particular set of equations and boundary conditions. And it is not probabilistic; everything is fixed by the deterministic dynamics, with no probabilistic assumptions on the velocity distributions or external stochastic forcing.

What new insights into spatio-temporal chaos or turbulence can the periodic-orbit theory provide? The theory yields accurate prediction for measurable time-averaged observables for a given geometry and Reynolds number, such as the mean frictional drag for the plane Couette flow (see figure 3), mean velocity profiles within the flow, or the mean pressure drop per unit length in a pipe flow. It offers a detailed qualitative and quantitative understanding of the geometry of turbulent vs. laminar basins of attraction, with applications to non-local control of such flows.

Suppose that the above program is successfully carried out for classical solutions of some field theory. What are we to make of this information if we are interested in the quantum behavior of the system?

2 Periodic orbit theory

Now we turn to the central issue; qualitatively, these solutions demonstrate that the recurrent patterns can be found, but how is this information to be used quantitatively? To quote the 1948 E. Hopf article [15]: *"The geometrical picture of the phase-space flow is, however, not the most important problem of the theory of turbulence. Of greater importance is the determination of the probability distributions associated with the phase-space flow."* This is the key challenge, the one in which the theory of dynamical systems has made the greatest progress in the last half century: the Sinai-Ruelle-Bowen ergodic theory of "natural" or SRB measures for far-from-equilibrium systems.

This part of the proposed research lies at the interface between pure mathematics on one side, and quantum mechanics and statistical physics on the other. The fundamental contributions on the mathematics side are due to Smale [16], Bowen [17], Sinai [18] and Ruelle [19]. Further excellent mathematical references are Parry and Pollicott [20], and Baladi [21, 22].

The proposed research involves difficult dynamical issues, in which the current mathematical work offers little guidance. This is a physics project, not pure mathematics, and the emphasis is not on rigor, but rather on experimentation and applicability of the theory. The fundamental contribution on the physics side is Gutzwiller's 1969-73 derivation of a semiclassical trace formula which expresses the quantum density of states as an infinite sum in terms of classical periodic orbits [23]. A key mathematics reference for generalizing these formulas to quantum field theory ("high-dimensional" Hamiltonian mechanics) is Arnol'd [24], while on the physics side monographs by Ozorio de Almeida [25], Brack and Bhaduri [26] and Gutzwiller [3] offer advanced introductions to semi-classical quantization.

Starting with the introduction of "cycle expansions" in 1988, PI and collaborators [27] have developed a unified approach to both the dynamical zeta functions of Ruelle and the semi-classical Zeta functions of Gutzwiller. The idea that chaotic dynamics is built upon unstable periodic orbits first arose in Ruelle's work on hyperbolic systems (not Poincaré), with ergodic averages associated with natural invariant measures expressed as weighted summations of the corresponding averages about the infinite set of unstable periodic orbits embedded in the underlying chaotic set. PI's contribution was to recast this theory in terms of highly convergent periodic-orbit expansions for which relatively few short periodic orbits led to high quality classical escape rates (for metastable systems) and quantal spectra for bound systems. Implementing PI's theory, the group of Wintgen obtained a surprisingly accurate helium spectrum [28] from a small set of shortest cycles, 50 years after failure of the old quantum theory to do so, and 20 years after Gutzwiller first introduced his quantization of chaotic systems.

In this theory contributions of different periodic orbits interfere and the quantization condition can no longer be attributed to a single periodic orbit: A coherent summation over the infinity of periodic orbit contributions gives the desired spectrum. The surprise was that the zeros of the dynamical zeta function derived in the context of classical chaotic dynamics,

$$1/\zeta(z) = \prod_p (1 - t_p) \,,$$

also yield excellent estimates of *quantum* resonances, with the quantum amplitude associated with a given cycle approximated semi-classically by the weight

$$t_p = \frac{1}{|\Lambda_p|^{\frac{1}{2}}} e^{\frac{i}{\hbar}S_p - i\pi m_p/2} \,, \tag{4}$$

whose magnitude is the square root of the classical weight

$$t_p = \frac{1}{|\Lambda_p|} e^{\beta\cdot A_p - \nu T_p} \,,$$

and the phase is given by the Bohr-Sommerfeld action integral S_p, together with an additional Maslov phase m_p, the number of caustics along the periodic trajectory, points where the naive semiclassical approximation fails. The quantal spectra of classically chaotic dynamical systems are determined from the zeros of dynamical zeta functions, defined by cycle expansions of infinite products of form

$$1/\zeta = \prod_p (1 - t_p) = 1 - \sum_f t_f - \sum_k c_k \tag{5}$$

with weight t_p associated to every prime (non-repeating) periodic orbit (or *cycle*) p.

PI's theory is based on the observation is that the chaotic dynamics is organized around a few *fundamental* cycles. These short cycles capture the skeletal topology of the motion in the sense that any long orbit can approximately be pieced together from the fundamental cycles. For this reason the cycle expansion (5) is a highly convergent expansion dominated by short cycles grouped into *fundamental* contributions, with longer cycles contributing rapidly decreasing *curvature* corrections.

The Kuramoto-Sivashinsky periodic orbit calculations of Lyapunov exponents and escape rates [8] demonstrate that the periodic orbit theory can be used to predict observable averages for deterministic but classically chaotic spatio-temporal systems.

However, the type of dynamics has a strong influence on the convergence of cycle expansions and the properties of quantal spectra; this necessitates development of different approaches for different types of dynamical behavior such as, on one hand, the strongly hyperbolic and, on the other hand, the intermittent dynamics. For generic non-hyperbolic systems, with mixed phase space and marginally stable orbits, periodic orbit summations are hard to control. *An importan part of the project will be to focus on incorporating intermittency (power-law) effects that arise in moderate-dimension Hamiltonian dynamics in problems such as hydrogen in crossed fields.*

3 Recurrent patterns: how to find them?

Sadly, searching for periodic orbits will never become as popular as a week on Côte d'Azur, or publishing yet another log-log plot in *Phys. Rev. Letters*. Writing a code to find even one unstable periodic orbit can take months for a novice, and there is no way to prepare a canned routine for all seasons - each dynamical system arrives with its own peculiarities and quirks. Although there has been much progresses in enumerating periodic orbits for many low-dimensional chaotic systems (mostly two-dimensional invertible maps or three-dimensional flows), obtaining a complete set of orbits for most systems in low or high dimensions remains a challenge.

The issue of *"how"* is an intensely numerical undertaking. Consider what is at stake: We need to compute, or extract from data, many distinct 3-dimensional color videos of patches of turbulence. Just in terms of memory we need something of order of a gigabyte to store a single pattern. That is still not so hard, but the theory proposed here seeks a 3-dimensional pattern that repeats itself *exactly* after a (yet to be determined) time period. *A priori*, we have no clue what such patterns look like, how big and what shapes are the basic spatial units, or what their time periods should be. So in our initial guess image *all* pixels are wrong, and we need to keep jostling them numerically until gigabytes of pixels settle into a pattern allowed by the laws of motion. Not only that, but a computer needs variable resolution, as small regions can play a very important role. All that takes computer time, lots of it. The theory then requires that we compute many such patterns, and be sure that we have found *all* of the patterns up to given spatial extent and time period within the desired tolerance limits.

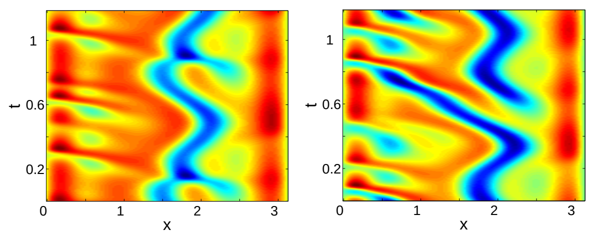


Figure 4: *A pattern and its near recurrence in a Kuramoto-Sivashinsky simulation: the swirl on the left recurs approximately within another pattern, right image. The color/greyscale codes the height of the flame front. [31]*

A variety of methods for determining all unstable periodic orbits up to a given length have been devised and successfully implemented for low-dimensional systems [27]. For turbulent flows, with high (or infinite) dimensional phase spaces and complicated dynamical behavior, most of the existing methods become unfeasible in practice. The bottleneck for the recurrent patterns program has been the lack of methods for finding even the simplest recurrent patterns, and the lack of intuition as to what such patterns would look like.

PI's Ph.D. student Y. Lan has formulated and explored numerically a novel variational principle for determining unstable spatio-temporally periodic solutions of extended systems [30, 31]. The idea of the method is to make a rough but informed guess of what the desired pattern looks like globally, and then use a variational method to drive the initial guess toward the exact solution. For robustness, we replace the guess of a single pattern at a given instant by a guess of an entire orbit. For numerical safety, we replace the Newton-Raphson iteration by the "Newton descent", a differential flow that strictly minimizes a cost function computed from the deviation of the approximate flow from the true flow.

3.1 Recurrent pattern searches

We make here a distinction between a *periodic orbit* — a low-dimensional trajectory that folds into itself after a time T, and a *recurrent pattern* — a trajectory in the infinite-dimensional state space $\mathcal{M}$ which tiles both space and time periodically. A periodic orbit is a solution (x, T) of the *periodic orbit condition* $f^T(x) = x$ for a given flow $x \to f^t(x)$. The task we face is to determine

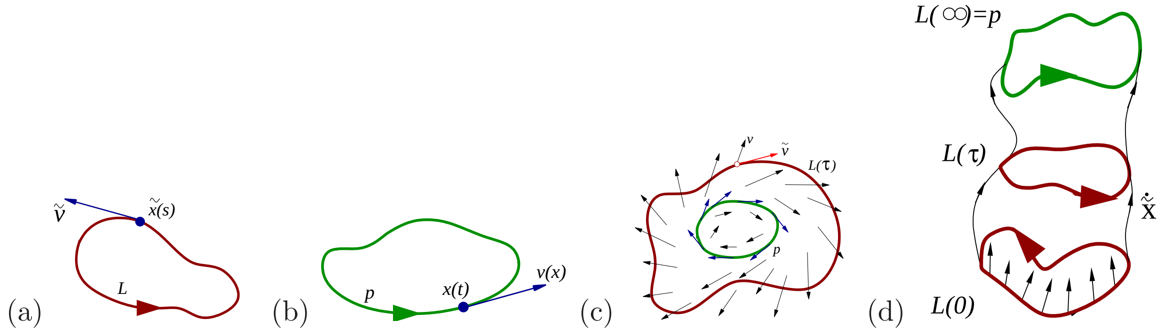


Figure 5: *(a) A loop L* defines *its tangent velocity vector $\tilde{v}$. (b) A periodic orbit p is* defined *by the vector field $v(x)$. (c) In general the orientation of the loop tangent $\tilde{v}(\tilde{x})$ does not coincide with the orientation of the velocity field $v(\tilde{x})$; for a periodic orbit p it does so at every $x \in p$. (d) An annulus $L(\tau)$ with the fictitious time flow $\dot{\tilde{x}}$ connecting smoothly the initial loop $L(0)$ to a periodic orbit p.*

a set of recurrent patterns of shortest periods. Any numerical solution of a PDE is based on its representation in terms of a truncated but large set of coupled nonlinear ODEs. So, in practice we always search for *periodic orbits* of flows defined by first order ODEs

$$\frac{dx}{dt} = v(x) \,, \qquad x \in \mathcal{M} \subset \mathbb{R}^d \tag{6}$$

in many dimensions d, with the vector field $v(x)$ a smooth, differentiable field.

We start by guessing a *loop*, a smooth, differentiable closed curve $\tilde{x}(s) \in L \subset \mathcal{M}$, parametrized by $s \in [0, 2\pi]$ with $\tilde{x}(s) = \tilde{x}(s + 2\pi)$, and the loop tangent vector

$$\tilde{v}(\tilde{x}) = \frac{d\tilde{x}}{ds} \,, \quad \tilde{x} = \tilde{x}(s) \in L \,.$$

The initial loop is *not* a solution of the flow equations — it is at best a rough guess as to what a solution might look like.

While there is no extremal principle associated with the general flow (6), at least three separate lines of argument (cost minimization [30], over-damped Newton method [31], Wiener-Onsager-Machlup stochastic path extremization [32]) all lead to the same variational principle, minimization of the cost function

$$F^2[\tilde{x}] = \frac{1}{|L|} \oint_L ds \, (\tilde{v} - v)^2 \,, \quad \tilde{v} = \tilde{v}(\tilde{x}(s, \tau)) \,, \;\; v = v(\tilde{x}(s, \tau)) \,, \tag{7}$$

which penalizes mis-orientation of the local loop tangent vector $\tilde{v}(\tilde{x})$ relative to the dynamical velocity field $v(\tilde{x})$ of (6), see figure 5 (c).

Vary the cost functional $F^2[\tilde{x}]$ with respect to the (yet undetermined) fictitious time τ,

$$\frac{dF^2}{d\tau} = \frac{2}{|L|} \oint_L ds \, (\tilde{v} - v) \frac{d}{d\tau} (\tilde{v} - v) \,.$$

The simplest, exponentially decreasing cost functional is obtained by taking the $\tilde{x}(s, \tau)$ dependence on τ to be point-wise proportional to the deviation of the two vector fields

$$\frac{d}{d\tau} (\tilde{v} - v) = -(\tilde{v} - v) \,, \tag{8}$$

so the fictitious time flow drives the loop to $L(\infty) = p$ monotonically, see figure 5 (d):

$$\tilde{v} - v = e^{-\tau}(\tilde{v} - v)|_{\tau=0} . \tag{9}$$

Making the $\tilde{x}$ dependence in (8) explicit we obtain the *Newton descent equation*, a PDE which evolves the initial loop $L(0)$ into the desired periodic orbit p in the fictitious time $\tau \to \infty$:

$$\frac{\partial^2 \tilde{x}}{\partial s \partial \tau} - A \frac{\partial \tilde{x}}{\partial \tau} = v - \tilde{v} , \qquad A_{ij}(x) = \frac{\partial v_i(x)}{\partial x_j} . \tag{10}$$

Numerically, we distribute many points along a smooth loop L (successive snapshots of the the pattern at successive time instants). The infinitesimal time step and loop deformation limit corresponds to this partial differential equation. In practice we do not need to solve this equation accurately along the way — only the periodic orbit itself needs to be computed with a high precision.

We initialize a search by long-time numerical runs of the dynamics, in order to limit the search to frequently visited regions of the phase space, *i.e.* the natural measure, and then search for close recurrences [33]. An initial loop guess $L(0)$ is crafted by taking a nearly recurring segment of the orbit, smoothed and made periodic by a FFT into the wavenumber representation, dropping the high frequency components, and an FFT back to the phase space.

PI's group has tested this new variational approach to finding recurrent patterns [30, 31] in detail on 1-*d* Kuramoto-Sivashinsky system, and several low-dimensional Hamiltonian systems. For these test examples many recurrent patterns have been successfully determined. *We plan to develop and deploy improved variational methods for recurrent pattern searches, in order to explore in detail the topology of moderate Reynolds number sustained steady turbulence attractors.*

4 Proposed research

The "recurrent patterns" approach to strongly nonlinear field theories is to visualize turbulence as a sequence of near recurrences in a repertoire of unstable spatio-temporal patterns. The investigations discussed above are first steps in the direction of implementing this program. If funded, this project would focus on following goals:

(1) Topology: In practice it is very hard to intuit what the solutions high-dimensional flows should look like. However, the preliminary investigations for intermediate size Kuramoto-Sivashinsky systems suggest that the strange attractors characterizing steady turbulence remain rather thin, and pieced together of repelling subsets similar to the strange attractor shown in figure 1, connected by rapid transitions between these subsets. In the language of unstable patterns, the system tries to maintain its typical mean wavelength by chaotic motion within a given wave number, followed by a rapid transition to another neirby wavenumber (pattern"defects"). Experimental and numerical observations suggest that this pictur applies also to 3-*d* shear flows such as the plane Couette flow. We shall use the short periodic orbits and their stability eigenvectors, eigenvalues and stable/unstable manifolds to piece together the asymptotic sttrange attractor(s) and construct approximate symbolic dynamics.

(3) Systems of infinite spatial extent: The dynamics over large space and time scales should be built up from small, computable patches of periodic solutions. So far, existence of a hierarchy of spatio-temporally recurrent patterns of a nonlinear field theory restricted to a small finite spatial intervals has been demonstrated, and the periodic orbit theory has been tested in evaluation of global averages for such system. But there is a big conceptual gap to bridge between what has been achieved, and what needs to be done: The system has been probed in its weakest turbulence regime. Numerical simulations demonstrate that as the viscosity decreases (or the size of the system increases), the “flame front” becomes increasingly unstable and turbulent. It is an open question to what extent the approach remains implementable as the system goes more turbulent. Preliminary forays (with C.P. Dettmann, and with Y. Lan, unpublished) in study of equilibria of the infinite extent Kuramoto-Sivashinsky system, and of periodic solutions of moderate size systems, give us confidence that a hierarchy of spatio-temporally periodic solutions can also be determined for systems of infinite spatial extent.

(4) A trace formula quantization of infinite dimensional systems: The Cvitanović-Eckhardt [29] classical trace formula has been successfully applied to dissipative extended systems. Given the successes of the periodic orbit theory for low-dimensional Hamiltonian systems, we are hopeful that it will work for a Hamiltonian field theory. As a key part of this proposal, a new semiclassical trace formula needs to be derived, a trace formula that combines Gutzwiller approach to unstable expanding directions with the Bohr-Sommerfeld quantization of the (infinity of) elliptically stable degrees of freedom of a Hamiltonian field theory. A preliminary exploration of hydrogen in crossed external fields (with Ph.D. student R. Paškauskas, unpublished), inspired by the work of PI's colleague T. Uzer and collaborators [34], suggests that such a formula exists, at least for finite-dimensional Hamiltonian problems.

4.1 Collaborative team

In part thanks to an unusually good crop of incoming Ph.D. students, and to the overall strength of the Georgia Tech nonlinear program, PI is in position to assemble a strong team to attack the above problems. The work proposed here will require 3 months per year of PI's research time, full time attention of 1 postdoctoral fellow, **Agapi Emmanouilidou** (CNS J. Ford fellow, current funding secured only for Oct. 2004 - Oct 2005) and 3 Georgia Tech Physics Ph.D. students: **D. Lippolis** (started Fall 2003) - “Generalized Gutzwiller trace formulas”, **J.E. Millan**, (started Fall 2003) - “Complex trajectories in semi-classical quantization”, and **R. Paškauskas** (started Fall 2000) - “Quantization on partially hyperbolic invariant tori”. Participation of Dr. Emmanouilidou, with her expertise in the Hamiltonian dynamics in higher dimensions, is essential to success of this project.

This proposal, whose emphasis on long time dynamics of high-dimensional Hamiltonian systems is motivated by problems of quantum theory and ergodic theory, is submitted to the NSF theoretical physics panel. In a parallel (many degrees-of-freedom) but distinct (dissipative, hence expect low-dimensional attracting sets) PI group's research effort, PI plans to work with 2 Georgia Tech Physics Ph.D. students, J.J. Halcrow (started Fall 2003) - “Plane Couette flow”, E. Siminos (started Fall 2003) - “Kuramoto-Sivashinsky turbulence”. and 2 external collaborators, V. Putkaradze (Mathematics, U. of New Mexico), and H.E. Johnston (Mathematics, U. of Massachusetts). PI is fortunate to have access to an exceptionally strong group of resident Georgia Tech *computational fluid dynamics* experts, in particular F. Sotiropoulos, School of Civil & Environmental Engineering and P.K. Yeung, School of Aerospace Engineering. This fluid-dynamics proposal will be submitted to the NSF applied dynamical systems panel.

4.2 Research plan

The proposed research mileposts:

Year 1: (a) **Variational searches for recurrent patterns:** Devise and implement an inversion of the loop linearized stability restricted to a finite inertial manifold subspace (regardless of the dimension of the discretized PDE truncation).

(b) **Kuramoto-Sivashinsky:** Test the variational code on 1-d Kuramoto-Sivashinsky flow for system sizes larger than those attained so far. The antisymmetric subspace (3) is unphysical, so explore the dynamics on the full space.

(c) **Symbolic dynamics:** Construct symbolic dynamics and approximate pruning rules for the above Kuramoto-Sivashinsky flow simulations, construct corresponding dynamical zeta functions, and compute expectation values of observables.

(d) **Plane Couette flow:** commence coding, testing the Navier-Stokes flow simulation code.

Year 2: (a) **Kuramoto-Sivashinsky:** study equilibrium solutions for the 1-d system of infinite extent. Use this information to classify types of spatially periodic structures.

(b) **Systems of infinite spatial extent:** implement a variational search method for recurrent patterns, compute a set of shortest such patterns in 1-d Kuramoto-Sivashinsky system.

(c) **Full trace formulas:** determine numerically partially hyperbolic invariant tori for hydrogen in crossed external fields or similar model problem.

Year 3: (a) **Plane Couette flow:** Search for a hierarchy of longer periodic orbits, and their linearized stability, eigenspectra and eigenvalues. Compute the frictional drag for a range of Re.

(b) **Full trace formulas:** derive a trace formula for combined hyperbolic - elliptic invariant surfaces, apply to hydrogen in crossed external fields, or a simple field theory, such as the nonlinear sigma model.

Intellectual Merit: A semi-classical quantization of any classically turbulent field theory by a Gutzwiller-type trace formula is a grand challenge for nonlinear dynamics. On the classical front, we already possess unique tools which we hope will lead to quantitatively precise deterministic predictive capabilities for turbulence, applicable to problems currently pursued in the engineering literature.

The point is, although the initial numerical computation required can be intensely time, memory and CPU consuming, once an approximate finite alphabet of patterns and a vocabulary of realizable short words (patterns explored sequentially by the dynamics) has been extracted - and this is done offline - the result is an alphabet of order of 100-1000 of patterns. The dynamics in terms of these patterns might be fast enough that it can be implemented in real time - a prerequisite for applying this theory to engineering problems, such as the turbulent drag control and reduction.

The impact of a major advance here is by no means restricted to hydrodynamical turbulence. The key concepts should be applicable to many systems extended in space, and a successful theory of spatially extended systems would have broad impact, from problems involving motions of fluids to subatomic phenomena to assemblies of neurons. *This proposal will address the grand challenge of nonlinear science: Explore experimentally and describe theoretically the dynamics of high-dimensional nonlinear systems.* In E. Hopf's own words: *The ultimate goal, however, must be a rational theory of statistical hydrodynamics where [$\cdots$] properties of turbulent flow can be mathematically deduced from the fundamental equations of hydromechanics.*

Broader impact: A modern education in the tools and methods of nonlinear science requires training that bridges traditional discipline boundaries. Students will acquire both the mathematical tools and develop physical intuition needed to tackle complex nonlinear problems arising in many different scientific fields. The Georgia Tech *Center for Nonlinear Science* [35] environment will complement the research component with a broad range of activities: interdepartmental research seminars, student-run seminars, an active visiting scientist program, and close interactions with Georgia Tech groups working on related problems, such as pattern formation and control, high-dimensional dynamics, coherent structures in turbulent flows. Collaborative visits to project partners (B. Eckhardt - Marburg, C.P. Dettmann - Bristol, G. Vattay - Budapest, G. Kawahara - Kyoto, and others) will provide additional training experience and opportunities, both domestic and abroad.

The outreach initiatives will include undergraduate research participation and an advanced nonlinear dynamics course. Currently under development by the `ChaosBook.org` cross-disciplinary team (particle physicists, mathematicians, nuclear physicists, condensed matter experimentalists and others), this novel hyper-linked web-based advanced graduate course [27] is already reaching students across the globe.

5 Prior, current and pending support

PI's quantum field theory contributions include evaluation of the sixth-order corrections to the electron magnetic moment (with T. Kinoshita), at the time the most demanding numerical computation in theoretical physics. A striking lesson of this long calculation were the amazing cancellations induced by gauge invariance. The desire to understand and exploit gauge invariance more effectively has motivated much of the subsequent research (including this proposal). The most interesting results of this effort were the mass-shell QCD Ward identities and the construction of the QCD gauge sets. This work motivated the formulation of planar field theory, rediscovered in 1994 by M.A. Douglas, D.J. Gross and R. Gopakumar, D.V. Voiculescu and others.

The studies of the QCD gauge invariance led to investigations of its group theoretical structure, and to the development of new methods for evaluating group-theoretic weights. This work led to the discovery of connections between various groups by continuations to negative dimensions, and to the construction of the magic triangle, a new construction of the Lie algebras which PI considers to be his most original work. A part of this has been rediscovered by Deligne in 1995 and is currently an active research topic in group theory.

PI's nonlinear dynamics contributions include the Feigenbaum-Cvitanović universal equation for period doubling [37], the theory of cycle expansions [27], and applications of the theory to systems that exhibit classical and quantum chaos.

Prior to moving to US, Cvitanović founded and directed in the period 1993-1998 *Center for Chaos and Turbulence Studies* (CATS) at the Niels Bohr Institute, Copenhagen, a cross-disciplinary effort which became one of Europe's leading centers for nonlinear science, housing and in part funding approximately 15 faculty, 8 post-docs, 45 graduate students, 15 long term visitors, 40 short term visitors, and 5 workshops/conferences in any given year.

PI is currently Glen Robinson Chair in Nonlinear Sciences and director of the newly created Georgia Tech *Center for Nonlinear Science* (CNS). In the period 1997-2000, prior to moving to GT, P. Cvitanović led the initiative to create a Center for Complex Systems at the Northwestern University, and was the original PI for **IGERT #9987577**: *Complex Systems in Science and Engineering program*, awarded to Northwestern for the period 2000-2004.