

Project Summary

We propose to describe spatio-temporally chaotic (turbulent) dynamics of strongly nonlinear quantum and classical field theories by means of an infinite hierarchy of spatio-temporally unstable recurrent patterns. The theory proposed is inspired by the unstable coherent structures observed in turbulence. For any finite spatial resolution, the system approximately tracks a pattern belonging to a repertoire of patterns, and the dynamics can be thought of as a walk through the space of such patterns. The dynamics over large space and time scales is built up from small, computable patches of periodic solutions, without recourse to statistical assumptions; this is a purely dynamic theory. The periodic orbit theory then yields the global averages characterizing the chaotic dynamics, as well as a starting semiclassical approximation to the quantum theory. Here new methods for computing quantum corrections to the semiclassical approximation need to be developed; in particular, we propose to implement nonlinear field transformations yielding the perturbative corrections in a form more compact than the Feynman diagram expansions.

Intellectual Merit: Turbulence is *the* unsolved problem of classical physics. Recent developments have greatly increased our insights in turbulence, and given us new concepts and modes of thought with far reaching repercussions in many different fields. However, there is a big conceptual gap to bridge between what has been achieved, and what needs to be done: So far, the recurrent patterns program has been implemented only on a very simple model, flutter of a flame front, and it is an open question to what extent the program remains viable as systems grow large and more turbulent. A systematic theory of spatio-temporal turbulence is *the* grand challenge of complex systems theory - how to deal with dynamics of very many degrees of freedom? A distinctive aspect of the proposed research is the integration of diverse areas of expertise: The problem of *how* to extract the recurrent patterns is an intensely numerical undertaking, a domain of fluid dynamicists. The proposed method for *what* to do with this infinity of patterns, periodic orbit theory, is domain of quantum theorists. We bring to this project both sets of skills, in an integration that is novel.

Broader Impact: The research proposed will be carried out at the Georgia Institute of Technology *Center for Nonlinear Science*, an interdisciplinary environment in which training of undergraduates, graduate students, and postdocs in relevant conceptual and numerical tools of the mathematics of complex systems is driven by concrete physical problems. The work will be carried out in collaboration with Profs. C.P. Dettmann, G. Vattay, V. Putkaradze and others in US and Europe. This type of international collaboration, with students sent to the other laboratory for extended collaboration periods, offers a unique environment for interdisciplinary training.

The theory of recurrent patterns that we propose to develop would by no means be restricted to quantum fields. The key concepts should be applicable to many systems extended in space, from motions of fluids to subatomic phenomena to assemblies of neurons. A successful theory of spatially extended systems would have broad impact: some of the examples of spatio-temporal turbulence to which the theory could be applied are few-particle molecular dynamics, nonlinear wave equations, fluid interfaces in oceanography and meteorology, chemical reactions, optic fibers, and Bose-Einstein condensates.

Project description: Chaotic Field Theory

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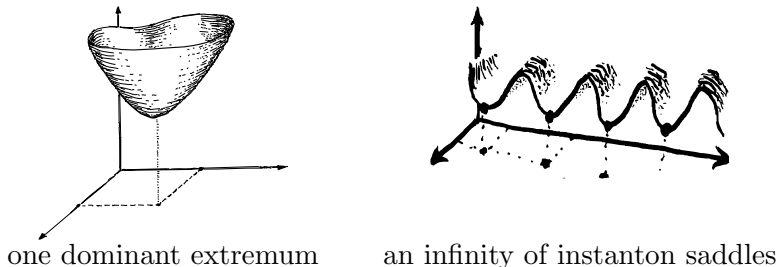
We start by sketching the challenge of a “Chaotic field theory,” and the need for a deeper understanding of classical turbulence that such theory presupposes. Then we illustrate the applicability of recurrent patterns program by an investigation of what perhaps is the simplest known example of turbulence, the Kuramoto-Sivashinsky system. We conclude by discussing what needs to be done.

1 Introduction

Formulated in 1946-49 and tested through 1970’s, quantum electrodynamics takes free electrons and photons as its point of departure, with nonlinear effects taken in account perturbatively in terms of Feynman diagrams, as corrections of order $(\alpha/\pi)^n = (0.002322819\dots)^n$. QED is a wildly successful theory, with Kinoshita’s [1] calculation of the electron magnetic moment agreeing with Dehmelt’s experiments [2] to 12 significant digits.

Quantum chromodynamics perturbative calculations seemed the natural next step, the only new feature being the gluon-gluon interactions. However, in this case the Feynman-diagrammatic expansions for observables such as the meson and hadron masses failed us utterly, perhaps because the expansion parameter is of order 1. We say perhaps, because more likely the error in this case is thinking in terms of quarks and gluons in the first place. Strongly nonlinear field theories require radically different approaches, and in 1970’s, with a deeper appreciation of the connections between field theory and statistical mechanics, their re-examination led to path integral formulations such as the lattice QCD [3]. 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. In the path integral formulation of a field theory the dominant contributions come from saddlepoints, the classical solutions of equations of motion. Usually one imagines one dominant saddle point, the “vacuum”:

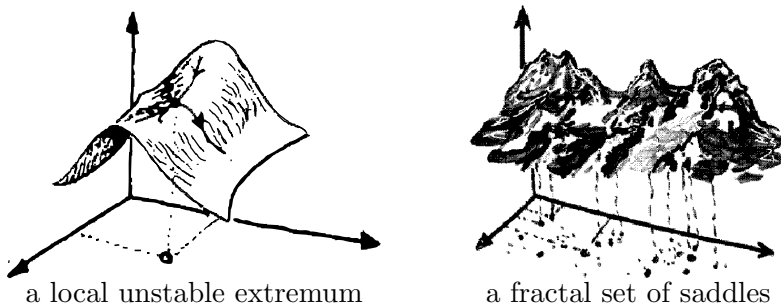


The Feynman diagrams of QED and QCD are nothing more than a scheme to compute the correction terms to this starting semiclassical, Gaussian saddlepoint approximation. But there might be other saddles. That field theories might have a rich repertoire of classical solutions became apparent with the discovery of instantons [4], analytic solutions of the classical $SU(2)$ Yang-Mills equations of motion, and the realization that the associated instanton vacua receive contributions from countable ∞ '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. In modern field theories the

main emphasis has been on symmetries as guiding principles in writing down the actions. 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 magnetohydrodynamics, the Ginzburg-Landau system — there should be very many solutions, with very few of the important ones analytical in form; the strongly nonlinear classical field theories are turbulent, after all. Furthermore, there is not a dimmest hope that such solutions are either beautiful or analytic, and there is not much enthusiasm for grinding out numerical solutions as long as one lacks ideas on what to do with them.

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 [5] in late 1960's. In this framework the spectrum of the theory is computed from a set of its unstable classical periodic solutions. The new aspect is that the individual saddles for classically chaotic systems are nothing like the harmonic oscillator degrees of freedom, the quarks and gluons of QCD — they are all unstable and highly nontrivial, accessible only by numerical techniques.

So, if one is to develop a semiclassical field theory of systems that are classically chaotic or “turbulent,” the problem one faces is twofold

- 1) determine and classify the classical solutions of nonlinear field theories.
- 2) develop methods for calculating perturbative corrections to these classical saddles.

In what follows we shall give an overview over the status of this program.

The first task, a systematic exploration of solutions of field theory, has so far been implemented only for one of the very simplest field theories, the 1-dimensional Kuramoto-Sivashinsky system. We sketch below how its spatio-temporally chaotic dynamics can be described in terms of spatio-temporally recurrent unstable patterns. For the second task, the theory of perturbative corrections, we shall turn to an even simpler system; a weakly stochastic mapping in 1-dimension. The new aspect of the theory is that now the corrections have to be computed saddle by saddle. In sect. 4.1 to sect. 4.3 we discuss three distinct methods for their evaluation.

2 Unstable recurrent patterns in classical field theories

Field theories such as 4-dimensional QCD or gravity have many dimensions, symmetries, tensorial indices. They are far too complicated for exploratory forays into this forbidding terrain. We start

instead by taking a simple spatio-temporally chaotic nonlinear system of physical interest, and investigate the nature of its solutions.

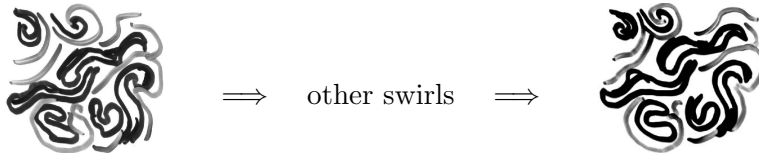
One of the simplest and extensively studied spatially extended dynamical systems is the Kuramoto-Sivashinsky system [6] (see Holmes, Lumley and Berkooz [8] for a delightful introduction to the subject):

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

which arises as an amplitude equation for interfacial instabilities in a variety of contexts, such as flame front. Amplitude $u(x, t)$ has compact support, with $x \in [0, 2\pi]$ 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. Numerical simulations demonstrate that as the viscosity decreases (or the size of the system increases), the “flame front” becomes increasingly unstable and turbulent. The task of the theory is to describe this spatio-temporal turbulence and yield quantitative predictions for its measurable consequences.

Armed with a computer and a great deal of skill, one can obtain a numerical solution to a nonlinear PDE. The real question is; once a solution is found, what is to be done with it? The periodic orbit theory is an answer to this question.

Dynamics drives a given spatially extended system through a repertoire of unstable patterns; as we watch a “turbulent” system evolve, every so often we catch a glimpse of a familiar pattern:



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 provides the machinery that converts this intuitive picture into a precise calculation scheme. For extended systems the theory gives a description of the asymptotics of partial differential equations in terms of recurrent spatio-temporal patterns.

We have proposed that the Kuramoto-Sivashinsky system (1) be used as a laboratory for exploring such ideas. We now summarize the published results obtained so far in this direction by Christiansen et al. [7] and Zoldi and Greenside [9].

The solution $u(x, t) = u(x + 2\pi, t)$ is periodic on the $x \in [0, 2\pi]$ interval, so one (but by no means only) way to solve such equations is to expand $u(x, t)$ in a discrete spatial Fourier series

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

Restrict the consideration to the subspace of odd solutions $u(x, t) = -u(-x, t)$ for which a_k are real. Substitution of (2) into (1) yields the infinite ladder of evolution equations for the Fourier coefficients a_k :

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

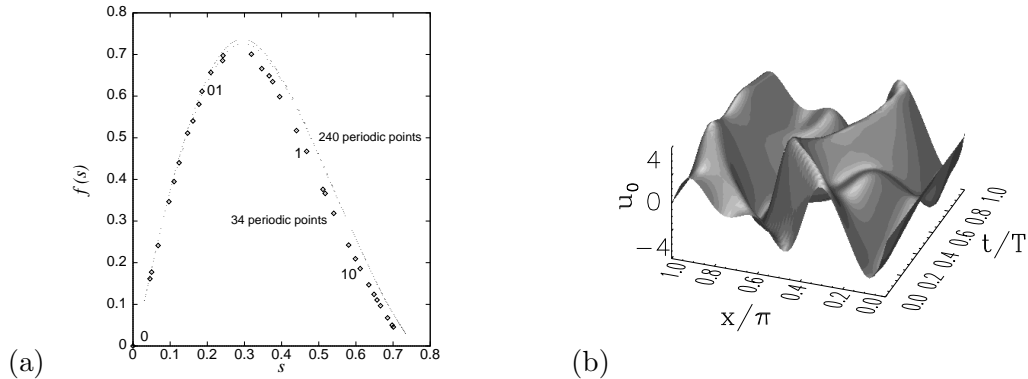


Figure 1: (a) The return map $s_{n+1} = f(s_n)$ constructed from periodic solutions of the Kuramoto-Sivashinsky equations (1), $\nu = 0.029910$, with s the distance measured along the unstable manifold of the fixed point $\bar{1}$. Periodic points $\bar{0}$ and $\bar{01}$ are also indicated. (b) One time period of the Spatio-temporally periodic solution $u_0(x, t)$ of the Kuramoto-Sivashinsky system, viscosity parameter $\nu = 0.029910$. From ref. [7].

$u(x, t) = 0$ 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. For $\nu > 1$, $u(x, t) = 0$ is the globally attractive stable fixed point; starting with $\nu = 1$ the solutions go through a rich sequence of bifurcations, and myriad unstable periodic solutions whose number grows exponentially with period.

The essential limitation on the numerical studies undertaken so far have been computational constraints: in truncation of high modes in the expansion (3), sufficiently many have to be retained to ensure the dynamics is accurately represented. Christiansen et al. [7] have examined the dynamics for values of the damping parameter close to the onset of chaos, while Zoldi and Greenside [9] have explored somewhat more turbulent values of ν . With improvement of numerical codes considerably *more turbulent regimes should become accessible, and will be investigated within the project proposed here.*

One pleasant surprise is that even though one is dealing with (infinite dimensional) PDEs, for strong dissipation values of parameters the spatio-temporal chaos is sufficiently weak that the flow can be visualised as an approximately 1-dimensional Poincaré return map $s \rightarrow f(s)$ from the unstable manifold of the shortest periodic point onto its neighborhood, see figure 1(a). This representation makes it possible to systematically determine all nearby periodic solutions up to a given maximal period.

So far some 1,000 prime cycles have been determined numerically for various values of viscosity. In figure 1(b) we plot $u_0(x, t)$ corresponding to the $\bar{0}$ -cycle. The difference between this solution and the other shortest period solution is of the order of 50% of a typical variation in the amplitude of $u(x, t)$, so the chaotic dynamics is already exploring a sizable swath in the space of possible patterns even so close to the onset of spatio-temporal chaos. Other solutions, plotted in the configuration space, exhibit the same overall gross structure. Together they form the repertoire of the recurrent spatio-temporal patterns that is being explored by the turbulent dynamics.

3 Theory of recurrent patterns

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? This is what the periodic orbit theory is about; it offers the machinery that assembles the topological and the quantitative information about individual solutions into accurate predictions about measurable global averages, such as the Lyapunov exponents and correlation functions.

Very briefly (for a detailed exposition consult refs. [11, 12]), the task of any theory that aspires to be a theory of chaotic, turbulent systems is to predict the value of an “observable” a from the spatial and time averages evaluated along dynamical trajectories $x(t)$

$$\langle a \rangle = \lim_{t \rightarrow \infty} \frac{1}{t} \langle A^t \rangle, \quad A^t(x) = \int_0^t d\tau a(x(\tau)).$$

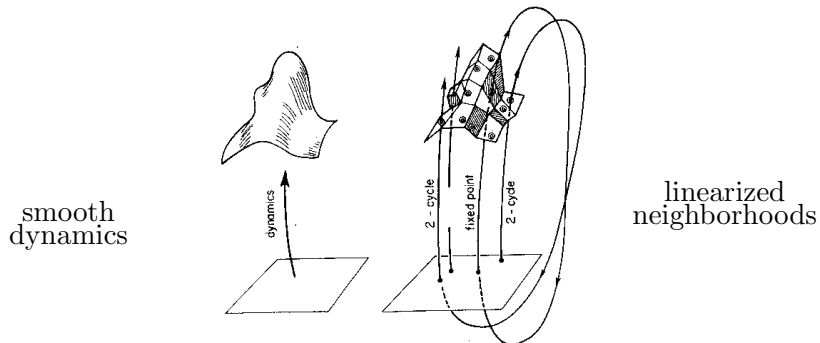
where $x(t)$ is a point in a high- (and in this context, infinite-) dimensional state space. The key idea of the periodic orbit theory is to extract this average from the leading eigenvalue of the evolution operator $\mathcal{L}^t(x, y) = \delta(y - x(t))e^{\beta A^t(x)}$ via the trace formula [10]

$$\text{tr } \mathcal{L}^t = \sum_p \text{ (spiral icon) } = \sum_p \sum_{r=1}^{\infty} \frac{T_p \delta(t - rT_p)}{|\det(\mathbf{1} - \mathbf{J}_p^r)|} e^{r\beta A_p} \quad (4)$$

which relates the spectrum of the evolution operator to a sum over prime periodic solutions p of the dynamical system and their repeats r .

What does this formula mean? Prime cycles partition the dynamical space into neighborhoods, each cycle enclosed by a tube whose volume is the product of its length T_p and its thickness $|\det(\mathbf{1} - \mathbf{J}_p)|^{-1}$. The trace picks up a periodic orbit contribution only when the time t equals a prime period or its repeat, a constraint enforced here by $\delta(t - rT_p)$. \mathbf{J}_p is the Jacobian of cycle p , so for long cycles $|\det(\mathbf{1} - \mathbf{J}_p^r)| \approx (\text{product of expanding eigenvalues})^r$, and the contribution of long and very unstable cycles are exponentially small compared to the short cycles which dominate trace formulas. The number of contracting directions and the overall dimension of the dynamical space is immaterial; that is why the theory also applies to (infinite-dimensional) PDEs. All this information is purely geometric, intrinsic to the flow, coordinate reparametrization invariant, and the same for any average one might wish to compute. The information related to a specific observable is carried by the weight $e^{\beta A_p}$, the periodic orbit estimate of the contribution of $e^{\beta A^t(x)}$ from the p -cycle neighborhood.

The intuitive meaning of a trace formula is that it expresses the average $\langle e^{\beta A^t} \rangle$ as a discretized integral

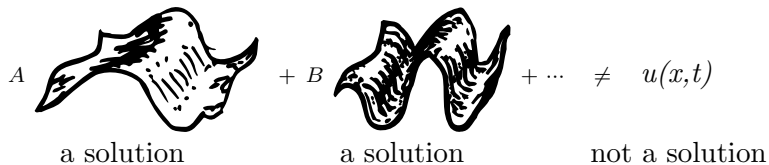


over the dynamical space partitioned topologically into a repertoire of spatio-temporal patterns, each weighted by the likelihood of pattern's occurrence in the long time evolution of the system.

Periodic solutions are important because they form the skeleton of the invariant set of the long time dynamics, with cycles ordered hierarchically; short cycles give dominant contributions to the invariant set, longer cycles corrections. Errors due to neglecting long cycles can be bounded, and for nice hyperbolic systems they fall off exponentially or even super-exponentially with the cutoff cycle length [13]. Short cycles can be accurately determined and global averages (such as Lyapunov exponents and escape rates) can be computed from short cycles by means of cycle expansions.

The Kuramoto-Sivashinsky periodic orbit calculations of Lyapunov exponents and escape rates [7] demonstrate that the periodic orbit theory can be used to predict observable averages for deterministic but classically chaotic spatio-temporal systems. In this particular application, the main problem is not how to compute such averages — periodic orbit theory as well as direct numerical simulations can handle that — but rather that there is no consensus on *what* the sensible experimental observables are worth predicting.

It should be obvious, and it still needs to be said: the spatio-temporally periodic solutions are *not* to be thought of as eigenmodes, a good linear basis for expressing solutions of the equations of motion. Something like a dilute instant approximation makes no sense at all for strongly nonlinear systems that we are considering here. As the equations are nonlinear, the periodic solutions are in no sense additive, and their linear superpositions are not solutions.



Instead, it is the trace formulas and spectral determinants of the periodic orbit theory that prescribe how the repertoire of admissible spatio-temporal patterns is to be systematically explored, and how these solutions are to be put together in order to predict measurable observables.

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? In the semiclassical quantization the classical solutions are the starting approximation.

4 Saddlepoint expansions for stochastic path integrals

For the same pragmatic reasons that we found it profitable to shy away from facing the 4-dimensional QCD head on in the above exploratory foray into a strongly nonlinear field theory, we shall start out by trying to understand the structure of perturbative corrections for systems radically simpler than a full-fledged quantum field theory. First, instead of perturbative corrections to the quantum problem, we shall start by exploring the perturbative corrections to weakly stochastic flows. Second, instead of continuous time flows, we shall start by a study of a discrete time process.

For discrete time dynamics a Langevin trajectory in presence of additive noise is generated by iteration

$$x_{n+1} = f(x_n) + \sigma \xi_n, \tag{5}$$

where $f(x)$ is a map, ξ_n a random variable, and σ parametrizes the noise strength. In what follows we assume that ξ_n are uncorrelated, and that the mapping $f(x)$ is one-dimensional and expanding,

but we expect that the form of the results will remain the same for higher dimensions, including the field theory example of the preceding section.

Tracking an individual noisy trajectory does not make much sense; what makes sense is the Fokker-Planck formulation, where one considers instead evolution of an ensemble of trajectories. An initial density of trajectories $\phi_0(x)$ evolves with time as

$$\phi_{n+1}(y) = (\mathcal{L} \circ \phi_n)(y) = \int dx \mathcal{L}(y, x) \phi_n(x) \quad (6)$$

where \mathcal{L} is the evolution operator

$$\mathcal{L}(y, x) = \int \delta(y - f(x) - \sigma\xi) P(\xi) d\xi = \sigma^{-1} P[\sigma^{-1}(y - f(x))], \quad (7)$$

and ξ_n a random variable with the normalized distribution $P(\xi)$, centered on $\xi = 0$.

If the noise is weak, the goal of the theory is to compute the perturbative corrections to the eigenvalues ν of \mathcal{L} order by order in the noise strength σ ,

$$\nu(\sigma) = \sum_{m=0}^{\infty} \nu^{(m)} \frac{\sigma^m}{m!}.$$

One way to get at the spectrum of \mathcal{L} is to consider the discrete Laplace transform of \mathcal{L}^n , or the resolvent

$$\sum_{n=1}^{\infty} z^n \text{tr} \mathcal{L}^n = \text{tr} \frac{z\mathcal{L}}{1 - z\mathcal{L}} = \sum_{\alpha=0}^{\infty} \frac{z\nu_{\alpha}}{1 - z\nu_{\alpha}} \quad (8)$$

which has a pole at every $z = \nu_{\alpha}^{-1}$.

The effects of weak noise are of interest in their own right, as any deterministic evolution that occurs in nature is affected by noise. However, what is most important in the present context is the fact that the form of perturbative corrections for the stochastic problem is the same as for the quantum problem, and still the actual calculations are sufficiently simple that one can explore many more orders in perturbation theory than would be possible for a full-fledged field theory, and develop new perturbative methods.

The first method we apply is the standard Feynman-diagrammatic expansion. For semiclassical quantum mechanics of a classically chaotic system such calculation was first carried out by Gaspard [14]. Our stochastic version [15] reveals features not so readily apparent in the quantum calculation.

The Feynman diagram method becomes unwieldy at higher orders. The second method, one that we have introduced in ref. [16], is based on Rugh's [13] explicit matrix representation of the evolution operator. If one is interested in evaluating numerically many orders of perturbation theory and many eigenvalues, this method is currently unsurpassed.

The third approach, the smooth conjugacies introduced by us in ref. [17], seems to be an altogether new idea in field theory. In this approach the neighborhood of each saddlepoint is rectified by an appropriate nonlinear field transformation, with the focus shifted from the dynamics in the original field variables to the properties of the conjugacy transformation.

4.1 Feynman diagrammatic expansions

We start our computation of the weak noise corrections to the spectrum of \mathcal{L} by calculating the trace of the n -th iterate of the stochastic evolution operator \mathcal{L} . A convenient choice of noise is

Gaussian, $P(\xi) = e^{-\xi^2/2}/\sqrt{2\pi}$, with the trace given by an n -dimensional integral on n points along a discrete periodic chain

$$\begin{aligned} \text{tr } \mathcal{L}^n &= \int dx_0 \cdots dx_{n-1} \mathcal{L}(x_0, x_{n-1}) \cdots \mathcal{L}(x_1, x_0) \\ &= \int [dx] \exp \left\{ -\frac{1}{2\sigma^2} \sum_a [x_{a+1} - f(x_a)]^2 \right\}, \quad x_n = x_0, \quad [dx] = \prod_{a=0}^{n-1} \frac{dx_a}{\sqrt{2\pi\sigma^2}}. \end{aligned} \quad (9)$$

The choice of Gaussian noise is not essential, as the methods that we develop here apply equally well to other noise distributions, and more generally to the space dependent noise distributions $P(x, \xi)$. As the neighborhood of any trajectory is nonlinearly distorted by the flow, the integrated noise is anyway never Gaussian.

If the classical dynamics is hyperbolic, periodic solutions of given finite period n are isolated. Furthermore, if the noise broadening σ is sufficiently weak they remain distinct, and the dominant contributions come from neighborhoods of periodic points, the tubes sketched in the trace formula (4). In the *saddlepoint approximation* the trace (9) is given by the sum over neighborhoods of periodic points

$$\text{tr } \mathcal{L}^n \longrightarrow \text{tr } \mathcal{L}^n|_{\text{sc}} = \sum_{x_c \in \text{Fix} f^n} e^{W_c} = \sum_p n_p \sum_{r=1}^{\infty} \delta_{n, n_p r} e^{W_{p^r}}. \quad (10)$$

As traces are cyclic, e^{W_c} is the same for all periodic points in a given cycle, independent of the choice of the starting point x_c , and the periodic point sum can be rewritten in terms of prime cycles p and their repeats. In the deterministic, $\sigma \rightarrow 0$ limit this is the discrete time version of the classical trace formula (4). Effects such as noise induced tunnelling are not included in the weak noise approximation.

We now turn to the evaluation of W_{p^r} , the weight of the r -th repeat of prime cycle p . The contribution of the cycle point x_a neighborhood is best expressed in an intrinsic coordinate system, by centering the coordinate system on the cycle points,

$$x_a \rightarrow x_a + \phi_a. \quad (11)$$

From now on x_a will refer to the position of the a -th periodic point, ϕ_a to the deviation of the noisy trajectory from the deterministic one, $f_a(\phi_a)$ to the map (5) centered on the a -th cycle point, and $f_a^{(m)}$ to its m -th derivative evaluated at the a -th cycle point:

$$f_a(\phi_a) = f(x_a + \phi_a) - x_{a+1}, \quad f'_a = f'(x_a), \quad f''_a = f''(x_a), \quad \cdots. \quad (12)$$

Rewriting the trace in vector notation, with x and $f(x)$ n -dimensional column vectors with components x_a and $f(x_a)$ respectively, expanding f in Taylor series around each of the periodic points in the orbit of x_c , separating out the quadratic part and integrating we obtain

$$\begin{aligned} e^{W_c} &= \int_c [d\phi] e^{-(\Delta^{-1}\phi - V'(\phi))^2/2\sigma^2} = \int_c [d\phi] e^{-\frac{1}{2\sigma^2} \phi^T \frac{1}{\Delta} \phi + (\cdots)} \\ &= |\det \Delta| \int_c [d\phi] e^{\sum \frac{1}{k} \text{tr}(\Delta V''(\phi))^k} e^{-\phi^2/2\sigma^2}. \end{aligned} \quad (13)$$

The $[n \times n]$ matrix Δ arises from the quadratic part of the exponent, while all higher powers of ϕ_a are collected in $V(\phi)$:

$$\Delta_{ab}^{-1} \phi_b = -f'_a \phi_a + \phi_{a+1}, \quad V(\phi) = \sum_a \sum_{m=2}^{\infty} f_a^{(m)} \frac{\phi_a^{m+1}}{(m+1)!}. \quad (14)$$

The saddlepoint expansion is most conveniently evaluated in terms of Feynman diagrams, by drawing Δ as a directed line, and the derivatives of V as the “interaction” vertices

$$\Delta_{ab} = \longrightarrow, \quad f_a'' = \longrightarrow \begin{array}{c} \nearrow \\ \searrow \end{array}, \quad f_a''' = \longrightarrow \begin{array}{c} \nearrow \searrow \\ \nwarrow \nearrow \end{array}, \quad \dots$$

In the language of field theory, Δ is the “free propagator”. Its determinant

$$|\det \Delta| = \frac{1}{|\Lambda_c - 1|}, \quad \Lambda_c = \prod_{a=0}^{n-1} f_a' \quad (15)$$

is the 1-dimensional version of the classical stability weight $|\det(\mathbf{1} - \mathbf{J})|^{-1}$ in (4), with Λ_c the stability of the n -cycle going through the periodic point x_c .

Standard methods [18] now yield the perturbation expansion in terms of the connected “vacuum bubbles”

$$W_c = -\ln |\Lambda_c - 1| + \sum_{k=1}^{\infty} W_{c,2k} \sigma^{2k} \quad (16)$$

$$W_{c,2} = \frac{1}{2} \begin{array}{c} \circlearrowleft \\ \bullet \\ \circlearrowright \end{array} \begin{array}{c} \longrightarrow \\ \bullet \\ \longrightarrow \end{array} \begin{array}{c} \circlearrowleft \\ \bullet \\ \circlearrowright \end{array} + \frac{1}{2} \begin{array}{c} \circlearrowleft \\ \bullet \\ \circlearrowright \end{array} \begin{array}{c} \longrightarrow \\ \bullet \\ \longrightarrow \end{array} \begin{array}{c} \circlearrowleft \\ \bullet \\ \circlearrowright \end{array} \begin{array}{c} \longrightarrow \\ \bullet \\ \longrightarrow \end{array} \begin{array}{c} \circlearrowleft \\ \bullet \\ \circlearrowright \end{array} + \frac{1}{2} \begin{array}{c} \circlearrowleft \\ \bullet \\ \circlearrowright \end{array} \begin{array}{c} \longrightarrow \\ \bullet \\ \longrightarrow \end{array} \begin{array}{c} \circlearrowleft \\ \bullet \\ \circlearrowright \end{array} \begin{array}{c} \longrightarrow \\ \bullet \\ \longrightarrow \end{array} \begin{array}{c} \circlearrowleft \\ \bullet \\ \circlearrowright \end{array} + \frac{1}{2} \begin{array}{c} \circlearrowleft \\ \bullet \\ \circlearrowright \end{array} \begin{array}{c} \longrightarrow \\ \bullet \\ \longrightarrow \end{array} \begin{array}{c} \circlearrowleft \\ \bullet \\ \circlearrowright \end{array}, \quad W_{c,4} = \dots$$

In the usual field-theoretic calculations the $W_{c,0}$ term corresponds to an overall volume term that cancels out in the expectation values. In contrast, as explained in sect. 3, here the $e^{W_{c,0}} = |\Lambda_c - 1|^{-1}$ term is the classical volume of cycle c . Not only does this weight not cancel out in the expectation value formulas, it plays the key role both in classical and semiclassical trace formulas.

In the diagrams sketched above a propagator line connects x_a at time a with x_b at later time b by a deterministic trajectory. At time b noise induces a kick whose strength depends on the local curvature of the flow. A penalty of a factor σ is paid, $m - 1$ deterministic trajectories originate in the neighborhood of x_b from vertex $V^{(m)}(x_b)$, and the process repeats itself, each vertex carrying a penalty of σ , and higher derivatives of the f_b . Summing over all noise kick sequences encoded by a given diagram, and using the periodicity of the trace integral (9), we obtain expressions such as [15]

$$\frac{r \Lambda_p^{2r} - 1}{2 \Lambda_p^2 - 1} \frac{\Lambda_p^r}{(\Lambda_p^r - 1)^3} \sum_{ab} \left(\frac{f_a''^2}{f_a'^2} - \frac{f_a'''}{f_a'} \right) \prod_{d=b+1}^{a-1} f_d'^2. \quad (17)$$

This particular sum is the value of the third Feynman diagram σ^2 correction to r -th repeat of prime cycle p in (16). More algebra leads to similar contributions from the remaining diagrams. But the overall result is surprising; the dependence on the repeat number r factorizes, with each diagram yielding the same prefactor depending only on Λ_p^r . This remarkable fact will be explained in sect. 4.3. The result of the Feynman-diagrammatic calculations is the *stochastic trace formula*

$$\text{tr} \frac{z\mathcal{L}}{1 - z\mathcal{L}} \Big|_{\text{sc}} = \sum_p \sum_{k=0}^{\infty} \frac{n_p t_{p,k}}{1 - t_{p,k}}, \quad t_{p,k} = \frac{z^{n_p}}{|\Lambda_p| \Lambda_p^k} e^{\frac{\sigma^2}{2} w_{p,k}^{(2)} + O(\sigma^4)}, \quad (18)$$

where $t_{p,k}$ is the k -th local eigenvalue evaluated on the p cycle. The deterministic, $\sigma = 0$ part of this formula is the stochastic equivalent of the Gutzwiller semiclassical trace formula [5]. The σ^2 correction $w_{p,k}^{(2)}$ is the stochastic analogue of Gaspard’s \hbar correction [14]. At the moment the explicit formula is sufficiently unenlightening that we postpone writing it down to sect. 4.3.

While the diagrams are standard, the chaotic field theory calculations are considerably more demanding than is usually the case in field theory. Here there is no translational invariance along the chain, so the vertex strength depends on the position, and the free propagator is not diagonalized by a Fourier transform. Furthermore, here one is quantizing neither around a trivial vacuum, nor a countable infinity of analytically explicit soliton saddles, but around an infinity of nontrivial unstable hyperbolic saddles, accessible only by highly non-trivial numerical calculations.

Two aspects of the above perturbative results are *a priori* far from obvious: (a) that the structure of the periodic orbit theory should survive introduction of noise, and (b) a more subtle and surprising result, repeats of prime cycles can be re-summed and theory reduced to the dynamical zeta functions and spectral determinants of the same form as for deterministic systems.

Pushing the Feynman-diagrammatic approach to higher orders is laborious, and has not been attempted for this class of problems. As we shall now see, it is not smart to keep pushing it, either, as one can compute many more orders of perturbation theory by means of a matrix representation for \mathcal{L} .

4.2 Evolution operator in a matrix representation

An expanding map $f(x)$ takes an initial smooth distribution $\phi(x)$ defined on a subinterval, stretches it out and overlays it over a larger interval. Repetition of this process smoothes the initial distribution $\phi(x)$, so it is natural to concentrate on smooth distributions $\phi_n(x)$, and represent them by their Taylor series. By expanding both $\phi_n(x)$ and $\phi_{n+1}(y)$ in (6) in Taylor series Rugh [13] derived a matrix representation of the evolution operator

$$\int dx \mathcal{L}(y, x) \frac{x^m}{m!} = \sum_{m'} \frac{y^{m'}}{m'!} \mathbf{L}_{m'm}, \quad m, m' = 0, 1, 2, \dots$$

which maps the x^m component of the density of trajectories $\phi_n(x)$ in (6) to the $y^{m'}$ component of the density $\phi_{n+1}(y)$ one time step later. The matrix elements follow by differentiating both sides with $\partial^{m'}/\partial y^{m'}$ and evaluating the integral

$$\mathbf{L}_{m'm} = \frac{\partial^{m'}}{\partial y^{m'}} \int dx \mathcal{L}(y, x) \frac{x^m}{m!} \Big|_{y=0}. \quad (19)$$

In (7) we have written the evolution operator \mathcal{L} in terms of the Dirac delta function in order to emphasize that in the weak noise limit the stochastic trajectories are concentrated along the classical trajectory $y = f(x)$. Hence it is natural to expand the kernel in a Taylor series [20] in σ

$$\mathcal{L}(y, x) = \delta(y - f(x)) + \sum_{n=2}^{\infty} \frac{(-\sigma)^n}{n!} \delta^{(n)}(y - f(x)) \int \xi^n P(\xi) d\xi, \quad (20)$$

where $\delta^{(n)}(y) = \frac{\partial^n}{\partial y^n} \delta(y)$. This yields a representation of the evolution operator centered along the classical trajectory, dominated by the deterministic Perron-Frobenius operator $\delta(y - f(x))$, with corrections given by derivatives of delta functions weighted by moments of the noise distribution $P_n = \int P(\xi) \xi^n d\xi$. We again center the coordinate system on the cycle points as in (11), and also introduce a notation for the operator (7) centered on the $x_a \rightarrow x_{a+1}$ segment of the classical trajectory

$$\mathcal{L}_a(\phi_{a+1}, \phi_a) = \mathcal{L}(x_{a+1} + \phi_{a+1}, x_a + \phi_a).$$

The weak noise expansion (20) for the a -th segment operator is given by

$$\mathcal{L}_a(\phi_{a+1}, \phi_a) = \delta(\phi_{a+1} - f_a(\phi_a)) + \sum_{n=2}^{\infty} \frac{(-\sigma)^n}{n!} P_n \delta^{(n)}(\phi_{a+1} - f_a(\phi_a)). \quad (21)$$

As the evolution operator has a simple δ -function form, the local matrix representation (19) of \mathcal{L}_a centered on the $x_a \rightarrow x_{a+1}$ segment of the deterministic trajectory can be evaluated recursively in terms of derivatives of the map f . The \mathbf{L}_a matrix elements are easily evaluated iteratively by computer algebra, with finite dimensional truncations to introducing exponentially small errors.

The trace formula (8) takes now a matrix form

$$\text{tr} \frac{z\mathcal{L}}{1 - z\mathcal{L}} \Big|_{\text{sc}} = \sum_p n_p \text{tr} \frac{z^{n_p} \mathbf{L}_p}{1 - z^{n_p} \mathbf{L}_p}, \quad (22)$$

where $\mathbf{L}_p = \mathbf{L}_{n_p} \cdots \mathbf{L}_2 \mathbf{L}_1$ is the contribution of the p cycle. The subscript sc is a reminder that this is a saddlepoint, or semiclassical approximation, valid as an asymptotic series in the limit of weak noise. Vattay [19] interprets the local matrix representation of the evolution operator as follows. The matrix identity $\log \det = \text{tr} \log$ together with the trace formula (22) yields

$$\det(1 - z\mathcal{L})|_{\text{sc}} = \prod_p \det(1 - z^{n_p} \mathbf{L}_p), \quad (23)$$

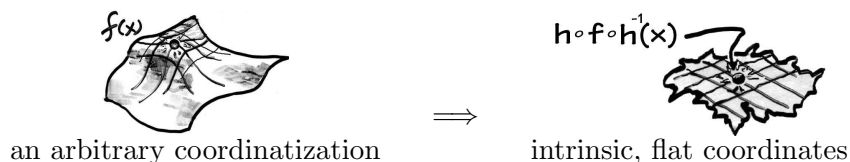
so in the saddlepoint approximation the spectrum of the *global* evolution operator \mathcal{L} is pieced together from the *local* spectra computed cycle-by-cycle on neighborhoods of individual prime cycles with periodic boundary conditions. The meaning of the k -th term in the trace formula (18) is now clear; it is the k -th eigenvalue of the local evolution operator restricted to the p -th cycle neighborhood.

Using this matrix representation Dettmann [25] was able to compute corrections to orders 64 (!) in noise strength, a feat simply impossible along the Feynman-diagrammatic line of attack. In retrospect, the matrix representation method for solving the stochastic evolution is eminently sensible — after all, that is the way one solves a close relative to stochastic PDEs, the Schrödinger equation. What is new is that the problem is being solved locally, periodic orbit by periodic orbit, by translation to coordinates intrinsic to the periodic orbit. It is this natural local basis that makes the matrix representation so simple.

In ref. [17] we take this observation one step further; as the dynamics is nonlinear, why not search for a nonlinear coordinate transformation that makes the intrinsic coordinates as simple as possible?

4.3 Smooth conjugacies

This step injects into field theory a method standard in the construction of normal forms for bifurcations [21]. The idea is to perform a smooth nonlinear coordinate transformation $x = h(y)$, $f(x) = h(g(h^{-1}(x)))$ that flattens out the vicinity of a fixed point and makes the map *linear* in an open neighborhood, $f(x) \rightarrow g(y) = \mathbf{J} \cdot y$.



The key idea of flattening the neighborhood of a saddlepoint can be traced back to Poincaré's celestial mechanics, and is perhaps not something that a field theorist would instinctively hark to as a method of computing perturbative corrections. This local rectification of a map can be implemented only for isolated non-degenerate fixed points (otherwise higher terms are required by the normal form expansion around the point), and only in finite neighborhoods, as the conjugating functions in general have finite radii of convergence.

We proceed in two steps. First, substitution of the weak noise perturbative expansion of the evolution operator (21) into the trace centered on cycle c generates products of derivatives of δ -functions:

$$\text{tr } \mathcal{L}^n|_c = \dots + \int [d\phi] \left\{ \dots \delta^{(m')}(\phi'' - f_a(\phi')) \delta^{(m)}(\phi' - f_{a-1}(\phi)) \dots \right\} + \dots .$$

The integrals are evaluated as in (19), yielding recursive derivative formulas such as

$$\int dx \delta^{(m)}(y) = \frac{1}{|y'(x)|} \left(-\frac{d}{dx} \frac{1}{y'(x)} \right)^m \Big|_{y=0}, \quad y = f(x) - x. \quad (24)$$

or n -point integrals, with derivatives distributed over n different δ -functions.

Next we linearize the neighborhood of the a -th cycle point. For a 1-dimensional map $f(x)$ with a fixed point $f(0) = 0$ of stability $\Lambda = f'(0)$, $|\Lambda| \neq 1$ we search for a smooth conjugation $h(x)$ such that:

$$f(x) = h(\Lambda h^{-1}(x)), \quad h(0) = 0, \quad h'(0) = 1. \quad (25)$$

In higher dimensions Λ is replaced by the Jacobian matrix \mathbf{J} . For a periodic orbit each point around the cycle has a differently distorted neighborhood, with differing second and higher derivatives, so the conjugation function h_a has to be computed point by point,

$$f_a(\phi) = h_{a+1}(f'_a h_a^{-1}(\phi)).$$

An explicit expression for h_a in terms of f is obtained by iterating around the whole cycle, and using the chain rule (15) for the cycle stability Λ_p

$$f_a^{n_p}(\phi) = h_a(\Lambda_p h_a^{-1}(\phi)), \quad (26)$$

so each h_a is given by some combination of f_a derivatives along the cycle. Expand $f(x)$ and $h(x)$

$$f(x) = \Lambda x + x^2 f_2 + x^3 f_3 + \dots, \quad h(y) = y + y^2 h_2 + y^3 h_3 + \dots,$$

and equate recursively coefficients in the functional equation $h(\Lambda y) = f(h(y))$ expansion

$$h(\Lambda u) - \Lambda h(u) = \sum_{n=2}^{\infty} f_n (h(u))^n. \quad (27)$$

This yields the expansion for the conjugation function h in terms of the mapping f

$$h_2 = \frac{f_2}{\Lambda(\Lambda - 1)}, \quad h_3 = \frac{2f_2^2 + \Lambda(\Lambda - 1)f_3}{\Lambda^2(\Lambda - 1)(\Lambda^2 - 1)}, \quad \dots \quad (28)$$

The periodic orbit conjugating functions h_a are obtained in the same way from (26), with proviso that the cycle stability is not marginal, $|\Lambda_p| \neq 1$.

What is gained by replacing the perturbation expansion in terms of $f^{(m)}$ by a perturbation expansion for the conjugacy function h ? Once the neighborhood of a fixed point is linearized, the conjugation formula for the repeats of the map

$$f^r(x) = h(\Lambda^r h^{-1}(x))$$

can be used to compute derivatives of a function composed with itself r times. The expansion for arbitrary number of repeats depends on the conjugacy function $h(x)$ computed for a *single* repeat, and all the dependence on the repeat number is carried by polynomials in Λ^r , a result that emerged as a surprise in the Feynman diagrammatic approach of sect. 4.1. The integrals such as (24) evaluated on the r -th repeat of prime cycle p

$$y(x) = f^{n_p r}(x) - x \tag{29}$$

have a simple dependence on the conjugating function h

$$\frac{1}{3!} \frac{\partial^2}{\partial y^2} \frac{1}{y'(0)} = \frac{\Lambda^r (1 + \Lambda^r)}{(\Lambda^r - 1)^3} (2h_2^2 - h_3) \tag{30}$$

The evaluation of n -point integrals is more subtle [17]. The final result of all these calculations is that expressions of form (30) depend on the conjugation function determined from the iterated map, with the saddlepoint approximation to the spectral determinant given by

$$\det(1 - z\mathcal{L}_\sigma)|_{sc} = \prod_p \prod_{k=0}^{\infty} (1 - t_{p,k})$$

in terms of local p -cycle eigenvalues

$$t_{p,k} = \frac{z^{n_p}}{|\Lambda_p| \Lambda_p^k} e^{\frac{\sigma^2}{2} P_2 w_{p,k}^{(2)} + \frac{\sigma^3}{3!} P_3 w_{p,k}^{(3)} + \frac{\sigma^4}{4!} P_4 w_{p,k}^{(4)} + O(\sigma^6)}$$

$$w_{p,k}^{(2)} = (k+1)^2 \sum_a (2h_{a,2}^2 - h_{a,3}), \quad w_{p,k}^{(3)} = \dots, \dots$$

accurate up to order σ^4 . $w^{(3)}$, $w^{(4)}$ are computed in ref. [17]. What is remarkable about these results is their simplicity when expressed in terms of the conjugation function h , as opposed to the Feynman diagram sums, in which each diagram contributes a sum like the one in (17), or worse. Furthermore, both the conjugation and the matrix approaches are easily automatized, as they require only recursive evaluation of derivatives, as opposed to the handcrafted Feynman diagrammar.

Simple minded as they might seem, discrete stochastic processes are a great laboratory for testing ideas that would otherwise be hard to test. Dettmann, Palla, Vattay, Voros and S ndergaard [22, 23, 24] have used a 1-dimensional repeller of bounded nonlinearity and complete binary symbolic dynamics to check numerically the above results, and computed the leading eigenvalue of \mathcal{L} by no less than five different methods; Dettmann [25] has carried this calculation to the first 64 orders(!) in noise strength. As anticipated by Rugh [13], the evolution operator eigenvalues converge super-exponentially with the cycle length; addition of cycles of period $(n+1)$ to the set of all cycles up to length n *doubles* the number of significant digits in the perturbative prediction. However, as the series is asymptotic, for realistic values of the noise strength summations beyond all orders are needed [24, 25].

5 Proposed research

The periodic orbit theory 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 three goals, attainable within the proposed 3-year framework.

1. 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 periodic solutions 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. The task of the theory is to describe this spatio-temporal turbulence and yield quantitative predictions for its measurable consequences. It is an open question to what extent the approach remains implementable as the system goes more turbulent. A preliminary exploration (with C.P. Dettmann, unpublished) of equilibria of the infinite extent Kuramoto-Sivashinsky system gives us confidence that a hierarchy of spatio-temporally periodic solutions can also be determined for systems of infinite spatial extent, and new, variational methods for determining recurrent patterns are currently under development [26, 27].

2. A trace formula quantization of infinite dimensional systems: The Cvitanović-Eckhardt [10] classical trace formula (4) has been successfully applied to dissipative extended systems. However, even though we are emboldened by other successes of the periodic orbit theory for low-dimensional Hamiltonian systems, we do not know whether it will work for a Hamiltonian field theory. And even if it works for classical Hamiltonian field theories, we do not know whether it will give us the quantum “chaotic field theory” sketched above. 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 (with my student R. Paskauskas, unpublished) inspired by the work of my colleague T. Uzer and collaborators [28], suggests that such a formula exists for finite-dimensional Hamiltonian problems.

3. Beyond Feynman-diagrammatic expansions: We have formulated a semiclassical perturbation theory for stochastic trace formulas with support on infinitely many chaotic saddles. The central object of the periodic orbit theory, the trace of the evolution operator, is a discrete path integral, like those found in field theory and statistical mechanics. The weak noise perturbation theory, likewise, resembles perturbative field theory, and can be cast into the standard field-theoretic language of Feynman diagrams. However, we found out that both the matrix and the nonlinear conjugacy perturbative methods are superior to the standard approach. In contrast to previous perturbative expansions around vacua and instanton solutions, the location and local properties of each saddlepoint must be found numerically.

The key idea in the new formulation of perturbation theory is this: Instead of separating the action into quadratic and “interaction” parts, one first performs a nonlinear field transformation which turns the saddle point into an exact quadratic form. The price one pays for this is the Jacobian of the nonlinear field transformation — but it turns out that the perturbation expansion of this Jacobian in terms of the conjugating function is order-by-order more compact than the

Feynman-diagrammatic expansion.

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 CNS 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 [29, 30, 31], such as pattern formation and control, high-dimensional dynamics, coherent structures in turbulent flows. Collaborative visits to project partners (C.P. Dettmann - Bristol, G. Vattay - Budapest, 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* cross-disciplinary team (particle physicists, nuclear physicists, condensed matter experimentalists and mathematicians), this novel hyper-linked web-based advanced graduate course [11] is already reaching students across the globe.

6 Prior, current and pending support

PI is currently Glen Robinson Chair in Nonlinear Sciences and director of the newly created Georgia Tech *Center for Nonlinear Science* (CNS). As a recent arrival to US, he has no NSF support. However, 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 on the **IGERT #9987577: *Complex Systems in Science and Engineering*** program, awarded to Northwestern for the period 2000-2004.

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.

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