

Actuation Requirements in High Dimensional Oscillator Systems

Bryan Eisenhower[†] and Igor Mezić[‡]

Abstract—Understanding actuation needs for re-conformation processes in high dimensional multi-stable systems is key to efficient nonlinear control design. Many solitary systems exhibit multiple equilibria and control of these systems when networked with others becomes a challenging task. In this paper we study a networked model in which each single entity contains multiple equilibria and an operational objective is to transition the entire coupled system from one equilibrium to another. We show that after a series of coordinate transformations, the structure of the system and mechanisms for internal resonance leading to this behavior become clear. We also characterize the amount of energy needed for such conformation change (the *activation energy*) both through numerical simulation and perturbation techniques. We find that unlike traditional Transition State Theories, the activation energy is a function of the spatial structure of such energy (it is not a constant number). We find that a reduced order model which results from averaging accurately predicts this activation energy in a very concise way.

I. INTRODUCTION

Directing systems with multistable potential energy landscapes to a single desired equilibria is a challenging task in nonlinear control theory. In addition, there is a clear trend in the control community towards controlling networked systems with a high number of entities or agents. If each of these entities possesses a nonlinear potential with multiple equilibria, actuation and control design becomes very complicated. In particular the task of changing the residence of the entire system from one region of attraction to another (*conformation change*) by means of energizing the system so as to breach a unstable saddle dividing different regions of attraction (*activation*) becomes a challenging problem with respect to both coordination and efficient actuation. The focus of this paper is to outline and present a tool for studying the robustness of such systems to external perturbation and a prediction algorithm for actuation requirements leading to conformation change.

Many systems contain multiple equilibria and at any given time only one of these equilibria is often desired. In biological systems multistability is an essential part of cellular function [1]. In this situation, macromolecules are often bound together with individual molecules connected as appendages off of a backbone-like structure. Different stable conformations exist dependent on how these appendages interact with other nearby molecules. In chemical systems, reaction kinetics follows a similar principle and as described

in introductory reaction texts, reactants and products exist on a potential landscape separated by a high energy saddle. Chemical reaction is realized when the energy of the species (containing many *agents*) exceeds the energy of this saddle allowing it to proceed to the other side of the potential. Similar behavior occurs in engineered settings such as control systems (see [2] for example). Autonomous search vehicles possess local control for avoidance (repulsion at close distances) and coordination (attraction at far distances) which is similar to a molecular potential. On a higher level, supervisory tasks may schedule the group of agents to switch between coordinate motion towards a search location, and a notably different motion upon arrival (chaotic search for example). Understanding the switching behavior between these two global equilibria is clearly important for sensitivity analysis and control authority specification. There is an abundance of other biological, chemical and physical systems which have functional concerns similar to these (e.g. extended power grids, neural systems, superconductor arrays, etc).

The transition of systems from one metastable state to another in a single dimension has been studied to great extent while in higher dimensions, the analysis is much more complex and the behavior is less understood. Although we intend this study to be applicable to general physical systems, we note that much of the ideas relating to the behavior discussed above has been studied under the premise of chemical reaction theory.

In chemical kinetics, the quantity of energy needed to switch a system between between states has been studied extensively in the past including a significant amount of work relating to rates of reaction in thermally equilibrated systems. These rate theories were initiated by Arrhenius over a century ago and developed further in the early 20th century using contributions from the work of fluctuation theory. It was these fluctuation theories and understanding of Brownian motion that opened a door to further understanding leading to Kramers rate theory (see a thorough review in [3]) which describes the mechanism of noise-assisted activation. It was Eyring in 1935 that solidified the idea of Transition State Theory (TST) which quantifies properties of reactive trajectories across a transition state primarily in unimolecular reactions. The general concept of these theories is that transitions in high dimensional systems occur when a single critical energy is surpassed which is determined from stochastic analysis of particle interactions.

Transition State Theory has been studied from a deterministic dynamical systems point of view in low dimensions while in higher dimensions only probabilistic understanding

[†]Student, Department of Mechanical and Environmental Engineering, University of California, Santa Barbara, CA

[‡]Professor, Department of Mechanical and Environmental Engineering, University of California, Santa Barbara, CA

is firmly understood. However, there has been some progress lately with the tools of Normally Hyperbolic Invariant Manifolds [4] to describe high dimensional energy barriers and the chaos that ensues (see the work of Stuart Rice, Turgay Uzer, Tamiki Komatsuxaki, Mikito Toda and others in the volume [5]). Very few studies have been performed on high dimensional deterministic systems, [6] investigates a system similar to ours while describing the behavior as dependent on transitory solitons which is a different situation than what we have here. Our research group has reported work that is similar to what is in this paper ([7] and [8]) while here we remove ourselves from the biological context and use a generic model with a cubic potential. We also present additional analysis that includes the use of averaging.

The essential mechanism for activation in high dimensional systems is internal energy transfer. In oscillatory systems energy transfer is most effective at resonance. For example, in a forced linear oscillator, maximal energy transfer will occur when the forcing frequency is tuned to the natural frequency of the open loop system. If the same system is autonomous, internal resonance occurs when internal frequencies are resonant (or commensurate) and therefore energy transfer is built into the design of the system. In nonlinear systems, where frequencies change within the phase space, the system may fall in and out of resonance as time proceeds. In this paper we investigate an example where this is indeed the case and perform parametric study of the impact of internal resonance on the activated response of the system.

To gain further insight into the energy transfer within these systems we study an example system with strong linear coupling and weak local nonlinearity. By a series of canonical coordinate transforms, we obtain a presentation of the system which illuminates its structure with respect to internal resonance. While accounting for the high dimension and multiple frequencies in this system we utilize averaging to obtain a reduced and approximate form. The reduced order model obtained from averaging highlights the interdependency of internal modes and how high order modes contribute to conformation change. The rest of the paper is organized in accordance with these steps and concludes with a summary of the results.

II. THE MODEL

To investigate the activation behavior of a high dimensional system we use multidimensional coupled oscillator model which contains local nonlinearity and strong coupling. This model has nonlinearity from a Duffing potential and linear coupling between nearest neighbors. This strong neighbor coupling acts like a *backbone* for the oscillator system. The dynamics are representative of many biological systems including coarse motion of macromolecules as well as other mechanical devices. As in these physical systems, the backbone has periodic boundary conditions (oscillators on a ring). Each oscillator possesses two stable equilibria at a symmetric distance on either side of the backbone which itself is an unstable equilibrium (at zero). Conformation

change is defined as the movement of all oscillators from one region of attraction to the other. The model consists of entirely conservative, deterministic dynamics and the constant Hamiltonian for this system containing N oscillators is:

$$\mathcal{H} = \sum_{k=1}^N \frac{p_k^2}{2} - \varepsilon \left(\frac{1}{2} q_{eq}^2 q_k^2 - \frac{1}{4} q_k^4 \right) + (q_{k-1} - q_k)^2 \quad (1)$$

where $(q_i, p_i) \in \mathbb{R} \times \mathbb{R}$ are position and conjugate momentum, q_{eq} specifies the position of the nonlinear equilibrium ($q_{eq} = 10$ for this study), and ε is a small parameter. The system is conservative and a contour plot of the constant energy levels for one oscillator is presented in Figure 1. Notice the two potential wells which map the two stable regions in the phase space of each bistable oscillator. This bistability is the key feature of the model that allows global conformation change. Different equilibria arise from both the nonlinear

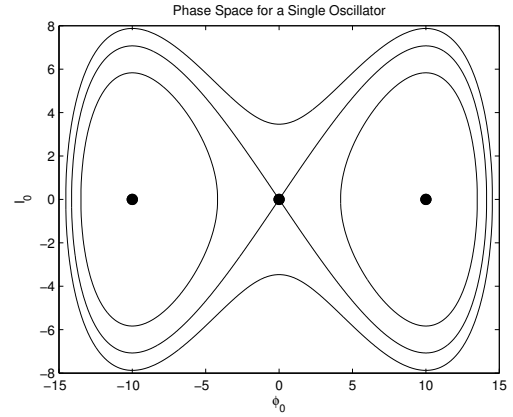


Fig. 1. Constant energy surface contours for a single oscillator with three equilibria denoted by black dots

and linear potentials, for the nonlinear potential there are three equilibria $q_i = \{0, \pm q_{eq}\}$ the first is unstable while the last two are linearly stable. The energy associated with each are $\{0, -\frac{\varepsilon q_{eq}^4 N}{4}, -\frac{\varepsilon q_{eq}^4 N}{4}\}$. The equilibria with respect to the neighbor interactions occurs when all oscillators are aligned collinearly. In summary, the global linearly stable equilibria is when all oscillators are aligned and at one of the two locations $(\pm q_{eq})$.

Numerous numerical experiments have been performed on Hamilton's equations (1) which illustrate that with even very modest initial displacement (in as few as one oscillator) it is possible that the entire system regresses to a collective behavior and re-conforms. The goal of this study is to illuminate the sensitivity of this system to external perturbation which invites this re-conformation behavior. In order to do this we perform a series of nonlinear (albeit canonical) coordinate transforms which reveal different aspects of the dynamics.

Because of the periodic boundary condition and translational invariance along the backbone, the spatial empirical eigenfunctions of this model are Fourier Modes [9]. To gain further insight into the dynamics along these coordinates we project the nominal model onto this basis using the normalized Discrete Fourier Transform (DFT). The projection

matrix (\mathcal{M}) for this procedure is a $N \times N$ linear orthogonal matrix which is a symplectic mapping between the original variables (\mathbf{q}, \mathbf{p}) and the modal coordinates $(\hat{\mathbf{q}}, \hat{\mathbf{p}})$ (the same matrix is used in [10]). The transformed coordinates and transformed Hamilton's equations take the form (bold characters refer to vectors):

$$(\hat{\mathbf{q}}, \hat{\mathbf{p}}) = (\mathcal{M}\mathbf{q}, \mathcal{M}\mathbf{p}) \rightarrow \left\{ \begin{array}{l} \dot{\hat{\mathbf{q}}} = \hat{f}(\hat{\mathbf{q}}, \hat{\mathbf{p}}) \\ \dot{\hat{\mathbf{p}}} = \hat{g}(\hat{\mathbf{q}}, \hat{\mathbf{p}}) \end{array} \right\} \quad (2)$$

With this transformation, we have organized the system into a single highly nonlinear mode (the zeroth mode, which is the average of all original oscillator positions) and a series nearly linear modes each representing a different spatial wavenumber (coupling still occurs between all modes). The nonlinear mode has one rank 1 saddle and a phase space is approximately equivalent to what is presented in Figure 1. This structure becomes more apparent in action-angle coordinates:

$$\begin{array}{l} \dot{\phi}_0 = I_0 \\ I_0 = 0 + \varepsilon g_0(\mathbf{I}, \phi, \varepsilon) \end{array} , \quad \begin{array}{l} \dot{\phi}_i = \omega_i + \varepsilon f_i(\mathbf{I}, \phi, \varepsilon) \\ I_i = 0 + \varepsilon g_i(\mathbf{I}, \phi, \varepsilon) \end{array} \quad (3)$$

where $(I_i, \phi_i) \in \mathbb{R} \times \mathbb{R}$ are the i^{th} action and angle and $\omega_i \in \mathbb{R}$ are the linear natural frequencies. Because of the nature of these coordinate transforms, high order spatial modes can be truncated without altering the structure of the dynamics or adding any dissipation. With this in mind, in the truncated model the indices follow nonzero wavenumbers $i = \{0, 1, 2, \dots, M\}$ and $M + 1 < N$ is defined as the dimension of this lower order model.

The transformed Hamiltonian is of the type which can be parsed into a zero-order regular Hamiltonian which is functional to only action and terms of small order ($O(\varepsilon)$). That is, the angle coordinates for all modes with nonzero wavelength are predominately linear and the action equations in linear limit are stationary. We also note at this point that the independent linear natural frequencies (ω_i) for each mode are not rationally commensurate and contain no spectral gap (for all realistic parameters). That is to say, the purely linear portion of the model, contains no resonance terms or significant time scale separation (however, this does not mean that the system never goes into resonance).

III. IDENTIFICATION OF INTERNAL RESONANCE

For the remainder of this paper we will discuss the behavior of the model presented above. In doing this, we will find that internal resonance is a significant contributor to the underlying dynamics and this is important because resonance is the doorway for energy transfer. Here we will briefly review the concepts and conditions of internal resonance in high dimensional oscillatory systems. The resonance conditions for a system with multiple frequencies ($\tilde{\omega}$) are [11]:

$$|(\boldsymbol{\kappa}, \tilde{\omega})| < \frac{1}{c|\boldsymbol{\kappa}|^v} \quad (4)$$

where $(\boldsymbol{\kappa}, \tilde{\omega}) = \kappa_0\tilde{\omega}_0 + \kappa_1\tilde{\omega}_1 + \dots + \kappa_{M-1}\tilde{\omega}_{M-1}$, κ_i are integers and c, v are positive constants. The quantity on the left hand side of the inequality goes to zero when frequencies

are rationally commensurate (exact resonance) and the term on the right hand side accounts for resonance in small regions where the frequencies are almost commensurate. In fact characteristics of the *resonance zone* both in the size of the region in phase space and time spent inside this region during evolution are related to this value. The resonance condition implies *internal resonance* when the system is autonomous (i.e. no external forcing).

Identifying whether resonance occurs becomes challenging when studying nonlinear systems. In linear fixed frequency systems, the condition (4) is evaluated once and the possibility of resonance is determined for all time. However, for nonlinear systems, whose frequencies change with amplitude of oscillation, this inequality may be satisfied only at specific times in the evolution. That is, the frequency for our nonlinear system is $\tilde{\omega}_i = \omega_i + \varepsilon f_i(\mathbf{I}, \phi, \varepsilon)$ (from equation 3) which varies with time. In our system, the vector containing $\omega'_i s$ is not commensurate, and so resonance only occurs with nonzero ε . That is, the term ε is a tuning knob that promotes internal resonance, and thus internal energy transfer which leads to efficient conformation change. This concept is important and will be explored with numerical simulation and averaging below.

IV. NUMERICAL SIMULATION

In this section we investigate activation behavior in a high dimensional Duffing system and internal resonance that enables it. To do this we present numerical simulations of the dynamics pointing out the structure of the system, cases of resonance, and the influence of the nonlinear perturbation term (ε) on its behavior. As described above, the system (3) is composed of one highly nonlinear mode and many nearly linear modes. This is confirmed by numerical simulation of the action-angle system by plotting the phase space of each individual mode. When doing this in a case where there is sufficient initial condition, the zeroth mode traverses a phase space similar to what is presented in Figure 1, and all other modes map out circles in the respected scaled phase spaces.

We also wish to study the influence of the small parameter ε on internal resonance in the system. One of the easiest ways to evaluate the resonance condition of Equation 4 is to simply probe the difference in frequencies between modes. Since we are interested in behavior of the zeroth mode, we investigate differences the frequency of this mode and other modes (we just look at the first 5 to keep things brief, though the trend continues through higher order modes). We find that at certain times, when there is sufficient nonlinear perturbation (in ε) this difference drops to zero which is indicative of resonance. Furthermore we see that in this case, the mostly circular trajectories of the nonzero modes become distorted which also represents internal energy transfer. This distortion occurs when the derivative of the difference in angles goes to zero.

In Figure 2 and 3 and we illustrate these behaviors with numerical simulation using $\varepsilon = 10^{-7}$ and $\varepsilon = 0.001$ respectively. All numerical simulations discussed in this paper were performed using a symplectic scheme to preserve

the Hamiltonian structure and avoid numerical dissipation [12]. The initial condition for the simulation is the rightmost equilibrium for the zeroth mode and equivalent action for all other nonzero modes. The amount of this action was adjusted such that there was sufficient energy to promote conformation change. The figures presented plot each phase space for the first 15 modes with the resonance condition described above with relation to time on the lowest subplot. We

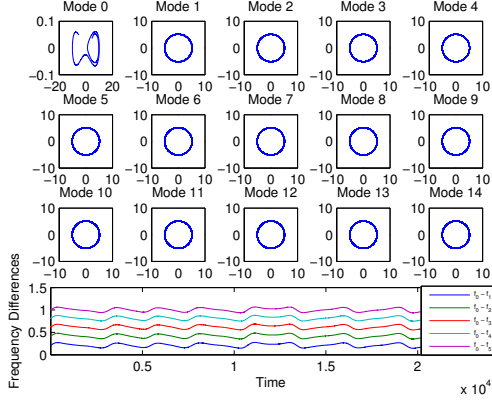


Fig. 2. Numerical simulation of the action-angle system with $\varepsilon = 10^{-7}$. Each upper subplot is a phase space of a mode while the lower subplot illustrates a resonance condition (f_i is equivalent to $\bar{\omega}_i$ as discussed in the text).

see that with the smaller value of nonlinear perturbation (Figure 2) the phase space of each nonzero mode remains nearly circular and that the frequency difference does not approach zero indicating very little resonance during the re-conformation process. On the other hand, with increased perturbation, we see this resonance condition dive towards zero frequently. In addition to this we find that the trajectories of the nonzero modes become distorted in their phase space which both indicate a high occurrence of internal resonance. The process of conformation change is leveraged by this internal resonance which is also evident in these numerical experiments. That is, the situation where resonance is negligible takes 24 times as long to re-conform with twice as much initial perturbation in action as the situation with stronger resonance.

V. AVERAGING

We now wish to have a deeper understanding of both the quality and quantity of energy needed for conformation change. In the numerical simulations above we provided data for a given initial amount of energy that was sufficient for conformation change. This energy was placed equally in all modes and increased in an *ad hoc* way until activation is realized. In this section we provide a tool to estimate the amount of actuation needed for the same behavior to occur. We do this by temporally averaging the Hamiltonian dynamics over the nonzero modes.

In our context, temporal averaging refers to approximating the dynamics by integrating their behavior over a periodic orbit. However, in our case we have a high dimensional system with multiple orbits of non commensurate frequency.

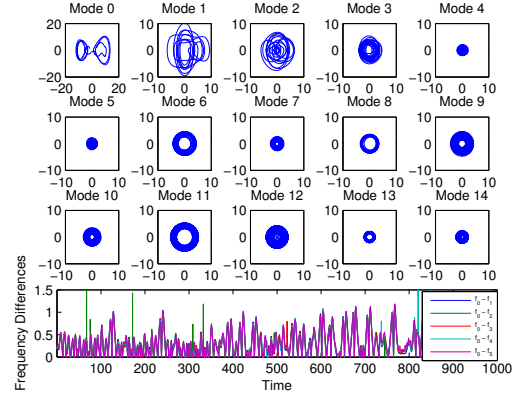


Fig. 3. Numerical simulation of the action-angle system with $\varepsilon = 0.001$. Each upper subplot is a phase space of a mode while the lower subplot illustrates a resonance condition.

Although this complicates the approach, systems of this type have been studied thoroughly in the past (see [11], [13], [14] or [15]). The basic way to accommodate these systems is to take the average over all angle variables:

$$\bar{\mathcal{H}}(\mathbf{I}) = \frac{1}{(2\pi)^M} \int_0^{2\pi} \dots \int_0^{2\pi} \mathcal{H}(\mathbf{I}, \phi, 0) d\phi_1 \dots d\phi_i \dots d\phi_M \quad (5)$$

where in our case we average over only the oscillatory modes ($i \neq 0$). The issue with this approach is that it does not represent the dynamics through resonance. Although there exists methods to average on each side of resonance and *splice* the two results together ([11], [16] and [17]) we choose to obtain the solutions only outside of resonance as they will turn out to be very insightful by themselves. With this in mind, we integrate over all of the higher order oscillatory dynamics which reveals reduced order action angle equations that capture the phase space outside of resonance (small ε). An example of the system when only one higher order mode (the i^{th} mode) is retained is:

$$\dot{\bar{I}}_0(t) = \varepsilon ((\hat{q}_{eq} - k_1 \bar{I}_i) \bar{\phi}_0(t) - k_2 \bar{\phi}_0(t)^3) \quad (6)$$

$$\dot{\bar{\phi}}_0(t) = \bar{I}_0(t) \quad (7)$$

$$\dot{\bar{I}}_i(t) = 0 \quad (8)$$

$$\dot{\bar{\phi}}_i(t) = f(\bar{I}_i(t), \bar{\phi}_0(t)) \quad (9)$$

Where k_1 and k_2 are constant coefficients including modal influences. Here we can see that in the averaged system, the actions from nonzero modes are stationary, and the phases from nonzero modes have no effect on the zeroth mode. That is, the effect of energy in the higher order modes is to reshape the phase space of the zeroth order mode. In fact, these values re-shape the phase space in a way that promotes activation and with this low order model we can estimate activation energies. As illustrated in Figure 1 the bistable phase space is separated by areas where the oscillator experience libration in one or the other potential well, as well as a foliation of manifolds in which rotation occurs. In the process of conformation change, the zeroth mode must enter

this path of rotation in order to proceed to the second well and this is the key to estimating activation energy.

VI. QUANTIFICATION OF ACTIVATION ENERGIES

With better understanding of the structure of the system with respect to energy transfer we now investigate required activation energy depending on the spatial structure in which energy is injected into the system. Two different quantities are investigated with respect to activation in the system; time needed for activation vs amount of energy injected into the system, and minimum amount of energy needed for activation. In the first case we perform a series of numerical experiments using the initial model (1) with $N = 30$ oscillators. In each simulation we impose initial potential energy onto one of the nonzero Fourier Modes (the zeroth mode is set to its equilibrium) and determine when the system breaches the high energy saddle which results in the entire oscillator chain moving from towards the second equilibrium.

The results for this experiment are presented in Figure 4 where we see two distinctive behaviors. First, it is clear that the amount of activation energy is dependent on spatial structure (Fourier Mode) of the initial potential energy and increases with the spatial wavenumber. This is important finding because most activation theories suggest a constant activation energy for any particular system. In addition to this we find that with very low energies, the amount of time needed for activation increases asymptotically. We call this asymptote the *minimum activation energy* and show that this is a well behaved function of the spatial structure of initial perturbation below. The minimum activation energy is

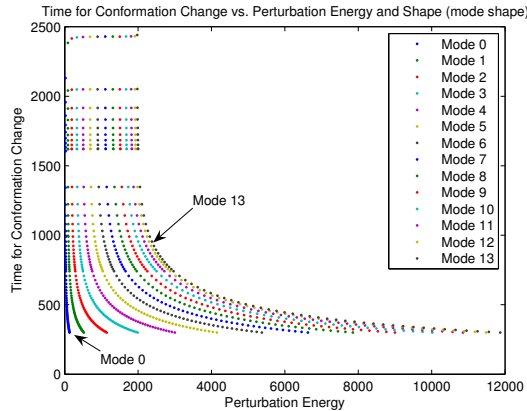


Fig. 4. Time for conformation change vs. energy imposed into one of the first 14 Fourier Modes ($\varepsilon = 1e - 7$)

a concept that is used in Transition State Theory of chemical kinetics, and as we have shown above varies with the type of energy driving the activation. Here we explore this further and show that this energy can be predicted by using the reduced order representation developed from averaging. The condition needed to cross the energy barrier is when the higher order actions drive the equilibrium of the zeroth mode across the separatrix between libration and rotation. If we

consider the potential energy of the system $\bar{U} = \bar{\mathcal{H}} - \bar{I}_0$ we have the condition for activation as:

$$\bar{U}(\hat{q}_0 = \hat{q}_{eq}, \bar{I}_1, \bar{I}_2, \dots, \bar{I}_M) = \bar{U}(\hat{q}_0 = 0.0, \bar{I}_1, \bar{I}_2, \dots, \bar{I}_M) \quad (10)$$

where \hat{q}_0 is modal coordinate representing the average of all angles, and \hat{q}_{eq} is one of the equilibrium positions (again, the barrier is 0.0). When energy is placed in a single mode, this condition reveals a single value of needed energy in this mode for activation. When energy is placed in multiple modes, this value is extended onto a affine hypersurface on which describes the needed activation energy depending on influence from any combination of higher order modes.

In Figure 5, we present and compare the minimum activation energy for the first five Fourier Modes with varying nonlinear perturbation (ε). One entry for each mode is from the averaging approach using the technique of condition (10), and the other entries are from numerical simulation. Note that in the condition derived from the averaging approach there is no effect from the small nonlinear perturbation. In each of the numerical simulation cases, the asymptotic value from the activation energy vs. time for activation curve is noted for each mode was noted for this plot (see Figure 4, more simulations were performed for other ε 's).

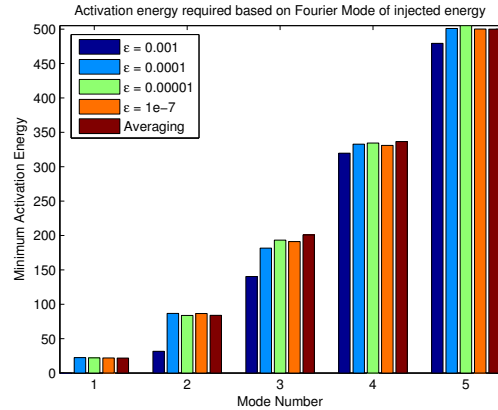


Fig. 5. Amount of activation energy needed for conformation change, as a result from long numerical simulation and prediction from a reduced order model obtained from averaging

From this plot we find that as expected, the results obtained from averaging agree with the cases of very low ε . As ε is increased the amount of activation energy predicted from averaging is greater than what is found in numerical simulation. This illustrates both the strength and limitations of using averaging for approximating the activation energy. A second characteristic which is nonintuitive but evident in this plot is that the amount of activation energy is a seemingly well behaved function of the Fourier Mode. In fact, it has been found that there exists an *activation invariant* with respect to the modal amplitudes in the system. Due to this, the activation energy becomes a nearly linear function of the temporal frequency of each Fourier Mode in which energy is imposed. This result is important as it reveals a very simple relation for predicting the actuation needs for re-conformation behavior in networked systems. The derivation

of this result is lengthy and is being prepared for a future publication.

VII. BIFURCATION BEHAVIOR

As we pointed out above, the influence from energy in higher order modes effects the zeroth mode by reshaping its phase space. The secondary effect of this is that a once stable equilibrium, which is surrounded by libration contours, eventually breaches the separatrix and ends up in the field of rotation. In fact, the influence of higher order modes is parametrically equivalent to inducing a pitchfork bifurcation on the phase space of the zeroth mode. Figure 6 illustrates the effect of action in one nonzero mode on the phase space of the zeroth mode. Notice that the original equilibrium at $\phi_0 = 10$ is initially surrounded by libration contours. However, upon increasing the action in the nonzero mode (\bar{I}_5) for this example, the equilibria are brought together and the location of this original equilibrium eventually is located in the field of rotation (for comparison, note that the minimum activation action for this mode is $I_5 = 500$). Eventually the equilibria coalesce at zero under a pitchfork bifurcation. The physical interpretation of this is that if energy is placed in this mode with a value greater than this bifurcation value, the system will continuously bounce back and forth between what used to be the original equilibria positions on either side of the backbone.

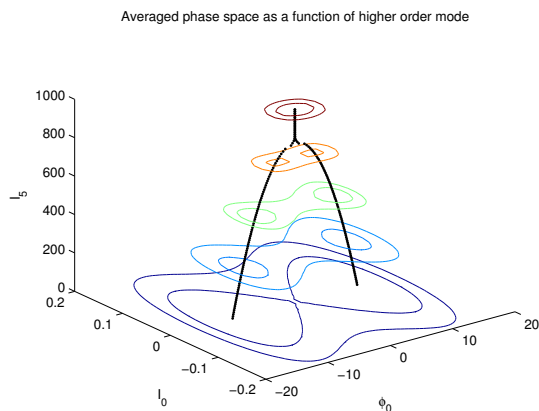


Fig. 6. Effect of energy in higher order modes on the zeroth mode illustrating with sufficient energy a pitchfork bifurcation occurs

VIII. SUMMARY

In this paper we have studied the activation behavior of a high dimensional multi-stable system. We have shown that unlike what is understood in traditional Transition State Theories, the activation energy is not single valued but rather a function of the structure of energy imposed on the system. We have presented results from a model that once analyzed after a series of canonical transformations supports these findings. With this model we have shown that the influence of higher order actions is to reshape the phase space of the lowest order mode which induces transition between equilibria. This effect can be captured by a reduced order model obtained from multi-frequency averaging. In fact, with

this low order model we find that higher order modes induce a pitchfork bifurcation of the phase space of the zeroth order mode. All of the work in this paper has been performed in a nonstatistical setting. The influence of noise and other environmental perturbation has been studied as well and it is found that that in the limit of low fluctuation, the results we present persist. The ability to have this low dimensional tool for prediction of actuation needs in a very high dimensional multi-agent system is beneficial to the design process for nonlinear control of such systems.

IX. ACKNOWLEDGEMENTS

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