

ANALYSIS OF OSCILLATORY BEHAVIOUR IN COUPLED DYNAMICAL SYSTEMS

SOUMYADIP BANERJEE



DEPARTMENT OF ELECTRICAL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY DELHI
OCTOBER 2021

© Indian Institute of Technology Delhi (IITD), New Delhi, 2021

All rights reserved.

ANALYSIS OF OSCILLATORY BEHAVIOUR IN COUPLED DYNAMICAL SYSTEMS

by

SOUMYADIP BANERJEE
Department of Electrical Engineering

Submitted

in fulfillment of the requirements of the degree of Doctor of Philosophy

to the



INDIAN INSTITUTE OF TECHNOLOGY DELHI
OCTOBER 2021

Imagination will often carry us to worlds that never were. But without it we go nowhere.

— Carl Sagan, *Cosmos*.

The thesis is dedicated to my mother and sister

CERTIFICATE

This is to certify that the thesis entitled **Analysis of Oscillatory Behaviour in Coupled Dynamical Systems** submitted by **Soumyadip Banerjee** to the Indian Institute of Technology Delhi, for the award of the Degree of **Doctor of Philosophy**, is a record of the bonafide research work carried out by him under my supervision and guidance. The thesis has reached the standards fulfilling the requirements of the regulations relating to the degree.

The results contained in this thesis have not been submitted either in part or in full to any other University or Institute for the award of any degree or diploma to the best of my knowledge.



Dr. Kushal Shah

Principal Data Scientist,

VuNet, Bangalore.

(Supervisor)



Prof. Shaunak Sen

Department of Electrical Engineering,

Indian Institute of Technology Delhi.

(Supervisor)

ACKNOWLEDGEMENTS

Getting an opportunity to study and do research at IIT Delhi has been one of the best things that has happened to my life. It has been a pleasant experience for me to work over here and be a part of this vibrant community. However, this journey would not have been possible if not for the constant support of my mentors, family and friends.

I would like to express my sincere gratitude to my supervisors, Dr. Kushal Shah and Prof. Shaunak Sen, to provide me with a strong foundation to do research work. Their constant guidance, support, and advice have always helped me choose the right path in my PhD journey. Also, I would like to give my deepest thanks to my Student Research Committee (SRC) members, Prof. S. Janardhan, Prof. I.N. Kar and Prof. A. Narang, for their valuable advice and feedback on my thesis work.

I would like to thank my lab members, Dr. Abhilash Patel, a close friend and a mentor, Dr. Venkat Bokka and Dr. Abhishek Dey, for all their help and support. Also, special thanks to Dr. Soumya Prakash Dash, Mrs. Jyoti Maheshwari, Mrs. Rakhi Sharma, Ms. Amita Giri and Mrs. Deepika Kumari for providing me with all the support and assistance at my working place. I cherish the beautiful moments spent with these lab mates.

I've also been fortunate to have some remarkable friends who have supported me throughout my journey. Special mention goes to Mr. Athar Kamal for being a dear friend and being available any time I needed him. I had with him innumerable discussions on various topics, primarily geeky topics! I would also like to thank Mr. Kamal Biswas, Mr. Jaswant Kumar Hirwani and Mr. Nitin Gupta for being such lovable friends. They were

always there to keep my spirits high and keep me motivated. I would also like to thank a dear friend of mine, Mrs. Bhaswati Chakraborty, who inspired me to take on this PhD journey. Also would like to thank Dr. Varun Saxena for all the advice and support he has given me as a friend.

Special gratitude goes to my family for always supporting me in my endeavours. Especially my mother, Mrs. Sikha Banerjee, for the selfless sacrifices she has given so that I can fulfil my dreams. I would always be indebted to her for all the love and moral support she has given to me in my hard times. Also, my heartiest gratitude to my sister, Ms. Soumita Banerjee, for her selfless love and support. Also, I offer my heartfelt gratitude to my other family members for their constant encouragement.

Lastly, I want to thank IIT Delhi for providing me with the facilities and a peaceful environment to do research work. On a final note, I thank the Visveswarya PhD scheme for providing me with all the financial support.

— Soumyadip Banerjee

Delhi

October 2021

ABSTRACT

Oscillatory dynamics explains various physical and biological phenomena in systems spanning different length scales, ranging from the microscopic scale of molecules to the macroscopic scale of biological and ecological systems. The mechanisms that drive these dynamics can be different in different systems. A useful approach to understand these mechanisms is to mathematically analyse the properties of a model representing the dynamics.

In this thesis, we use averaging methods to study oscillatory dynamics in three problems. The first is to analyse the collective dynamics of a periodically driven collisionless non-neutral plasma, which is usually modelled using ponderomotive theory, which in turn is generally derived using heuristic methods. By applying Hamiltonian averaging theory on the Vlasov equation, we have rigorously derived the time-averaged distribution function predicted by ponderomotive theory, and clearly showed that the ponderomotive solution is only one among the infinitely many different solutions possible. We have also analysed various initial conditions which can lead to periodic solutions of the Vlasov equation for such plasmas and conjectured that the irreducible polynomial corresponding to the initial plasma distribution function must only have squares of the spatial and momentum coordinates. The time-dependent plasma distribution function for all other initial conditions is likely to be aperiodic and can lead to complex relaxation processes within the plasma. The second is in the context of understanding the conformational change of a DNA molecule. The phenomenon is important to various biological processes and is often modelled using a chain of linearly coupled oscillators subjected to a weak non-linear perturbation. Several reduced-order models derived using averaging techniques have been used to investigate the full model's conformational dynamics; however, the influence of chain length on this dynamics is relatively less clear. These reduced-order models are

based on an important approximation, i.e., the full system's nonzero modes follow the unperturbed dynamics. We examined this approximation by calculating the perturbed modal frequency of a nonzero mode both using a modified Lindstedt-Poincare method and numerical computations. We found that the approximation on which the previous reduced-order models are based may fail to hold when the chain length is large. The third is in the context of understanding the robustness of a biomolecular oscillator to transient perturbations. Biomolecular oscillators are known to operate robustly in the presence of environmental perturbations. Although the influence of circuit parameters and the mechanisms underlying the oscillator's robustness to steady perturbations have been investigated, the scenario for dynamic perturbations is relatively less clear. To address it, we first investigated the use of an averaging technique to predict the short term response of a stable limit cycle model of a biomolecular oscillator subjected to an initial condition perturbation. The application of Floquet theory was tested and was found to provide a valid prediction because of a good correlation between the time scale of the short term response obtained using the full model simulation and the time scale predicted by Floquet theory. Further, a metric derived from the Floquet time scale was used to identify the oscillator's intrinsic and structural features, which can improve the oscillator's short-term response.

These studies would help to understand better the use of averaging methods in studying oscillatory dynamics.

सार

ऑसिलेटरी डायनामिक्स विभिन्न लंबाई के पैमानों में फैली प्रणालियों में विभिन्न भौतिक और जैविक घटनाओं की व्याख्या करता है, जिसमें अणुओं के सूक्ष्म पैमाने से लेकर जैविक और पारिस्थितिक प्रणालियों के मैक्रोस्कोपिक पैमाने तक शामिल हैं। इन गतिकी को चलाने वाले तंत्र विभिन्न प्रणालियों में भिन्न हो सकते हैं। इन्हें समझने का एक उपयोगी तरीका तंत्र गतिकी का प्रतिनिधित्व करने वाले मॉडल के गुणों का गणितीय विश्लेषण करना है।

इस थीसिस में, हम तीन समस्याओं में ऑसिलेटरी डायनामिक्स का अध्ययन करने के लिए औसत तकनिक का इस्तेमाल किया है। पहले हमने, समय-समय पर संचालित गैर-तटस्थ प्लाज्मा का सामूहिक गतिशीलता का विश्लेषण किया है, जिसे आमतौर पर पॉन्डरोमोटिव सिद्धांत का उपयोग करके मॉडल किया जाता है। प्लाज्मा समीकरण पर हैमिल्टोनियन के औसत तकनिक को लगा कर हमने पॉन्डरोमोटिव सिद्धांत द्वारा अनुमानित समय-औसत वितरण फ़ंक्शन को प्राप्त किया है और स्पष्ट रूप से दिखाया है कि पॉन्डरोमोटिव समाधान असीम रूप से कई संभावित समाधानों में से एक है। हमने विभिन्न प्रारंभिक स्थितियों का भी विश्लेषण किया है जो ऐसे प्लाज्मा के लिए प्लाज्मा समीकरण के आवधिक समाधान का कारण बन सकता है और अनुमान लगाया गया है कि प्रारंभिक प्लाज्मा वितरण फ़ंक्शन के अनुरूप इरेड्यूसिबल बहुपद में केवल स्थानिक और गति निर्देशांक के वर्ग होने चाहिए। अन्य सभी प्रारंभिक स्थितियों के लिए समय-निर्भर प्लाज्मा वितरण समारोह एपेरियोडिक होने की संभावना है और प्लाज्मा के भीतर जटिल विश्राम प्रक्रियाओं को जन्म दे सकता है। दूसरा एक डीएनए अणु के गठनात्मक परिवर्तन को समझने के संदर्भ में है। यह घटना विभिन्न जैविक प्रक्रियाओं के लिए महत्वपूर्ण है। अक्सर एक कमजोर गैर-रैखिक विचलन के अधीन रैखिक रूप से युग्मित दोलकों की एक श्रृंखला का उपयोग करके मॉडलिंग की जाती है। औसत तकनीकों का उपयोग करके व्युत्पन्न कई कम-क्रम वाले मॉडल रहे हैं जिसका पूर्ण मॉडल के गठनात्मक गतिकी की जांच करने के लिए उपयोग किया जाता है; हालाँकि, इस गतिकी पर श्रृंखला की लंबाई का प्रभाव आंशिक रूप से कम स्पष्ट है। ये कम-क्रम वाले मॉडल एक महत्वपूर्ण सन्निकटन पर आधारित होते हैं, अर्थात्, पूर्ण सिस्टम के गैर-शून्य मोड अप्रभावित गतिकी का अनुसरण करते हैं। हमने संशोधित लिंडस्टेड-पोइनकेयर विधि और संख्यात्मक संगणना का उपयोग करके एक गैर-शून्य मोड की विकृत मोडल आवृत्ति की गणना करके इस

सन्निकटन की जांच की है। हमने पाया कि, जिस सन्निकटन पर कम-आदेश मॉडल आधारित हैं, वह श्रृंखला की लंबाई बढ़ी होने पर विफल हो सकता है। तीसरा क्षणिक विचलन के प्रतिकूल जैव-आणविक ऑसिलेटर की मजबूती को समझने के संदर्भ में है। बायोमोलैक्यूलर ऑसिलेटर्स पर्यावरणीय विचलन के रहते हुए भी काम कर सकती है। हालांकि सर्किट मापदंडों के प्रभाव और स्थिर गड़बड़ी के लिए ऑसिलेटर की मजबूती के अंतर्निहित तंत्र की जांच की गई है, गतिशील विचलन के खिलाफ मजबूती आंशिक रूप से स्पष्ट है। इसे संबोधित करने के लिए, हमने पहले एक प्रारंभिक स्थिति के अधीन एक जैव-आणविक ऑसिलेटर के एक स्थिर सीमा चक्र मॉडल की अल्पकालिक प्रतिक्रिया की भविष्यवाणी करने के लिए एक औसत तकनीक का उपयोग किया। हमने यहां फ्लोकेट सिद्धांत लागू होता है कि नहीं विश्लेषण किया। हमें फ्लोकेट सिद्धांत से प्राप्त मीट्रिक और अल्पावधि के समय के पैमाने के बीच एक अच्छे संबंध मिला। आगे हमने फ्लोकेट टाइम स्केल से प्राप्त एक मीट्रिक का उपयोग ऑसिलेटर की आंतरिक और संरचनात्मक विशेषताएं को पहचानने के लिए किया जो ऑसिलेटर की अल्पकालिक प्रतिक्रिया में सुधार कर सकती हैं।

इन अध्ययनों से ऑसिलेटरी डायनामिक के अध्ययन में औसत विधियों के उपयोग को बेहतर ढंग से समझने में मदद मिलेगी।

Contents

List of Figures	ix
List of Tables	xi
1 Introduction	1
1.1 Averaging methods	4
1.2 Applications	9
1.2.1 A periodically driven system	9
1.2.2 Floquet theory	12
1.3 Contributions of the thesis	16
2 Vlasov dynamics of periodically driven systems	18
2.1 Vlasov equation	19
2.2 Ponderomotive theory	24
2.3 Periodic solution	30
2.4 Condition for periodicity	37
2.5 Discussion	40
3 Conformational behaviour of a biomolecule	43
3.1 DNA Model	45
3.2 Flipping as a change in conformation	48

3.3	Dynamics in Fourier space	52
3.3.1	Unperturbed modes	52
3.3.2	Perturbed modes	55
3.4	Flipping mechanism	56
3.5	Flipping behaviour as a function of length	61
3.6	Discussion	68
4	Transient response in a biomolecular oscillator	73
4.1	Oscillator model	75
4.2	Settling time of transient response	77
4.3	How to improve settling time?	79
4.4	Discussion	85
5	Summary and Future directions	88
5.1	Summary	88
5.2	Future directions	91
	Bibliography	94
	Appendix A	113
A.1	Method of characteristics	113
A.1.1	Solving linear-advection equation	113
	Appendix B	116
B.1	Transformation from real to modal co-ordinates	116
B.1.1	Transformation matrix	116
B.1.2	Eigenvalues of the linear system	118
B.2	Perturbed modal frequency	120

Appendix C	126
C.1 Floquet settling time	126
C.2 Transient response in a repressilator variant	128
Publications	136
BIO-DATA	137

List of Figures

1.1	Mechanism behind oscillations	3
1.2	Using averaging methods to predict long-term oscillatory behaviour	7
1.3	Averaged dynamics of a Linear Time-Periodic (LTP) system	14
2.1	Flow of a collision-less plasma	21
3.1	DNA molecule represented as a chain of coupled pendula under the influence of a bi-stable potential	47
3.2	Flipping phenomena in a DNA model subjected to local perturbation	50
3.3	Resonance between modes may influence flipping in DNA model	57
3.4	Reduced order model may not hold in DNA model having large lengths	59
3.5	Flipping properties depends on length of the model	63
3.6	Tendency towards flipping increases with length of the DNA system when subjected to random perturbation	67
4.1	Illustration of an oscillator's robustness to pulse perturbation	76
4.2	Oscillatory behaviour of a repressilator model	76
4.3	Dominant Floquet multiplier as a measure of robustness to pulse perturbation	78
4.4	Robustness to pulse perturbation depends on the choice of intrinsic parameters	81

4.5	Structural modifications in repressilator can improve its robustness to pulse perturbation	83
C.1	Repressilator variant	130
C.2	Settling time for different feedback strengths (data provided for pulse perturbation to two parameters)	134
C.3	Settling time for different feedback strengths (data provided for pulse perturbation to rest of parameters)	135

List of Tables

C.1	Metrics for pulse perturbation applied to oscillator without feedback	131
C.2	Metrics for pulse perturbation applied to oscillator with negative feedback	133
C.3	Metrics for pulse perturbation applied to oscillator with positive feedback .	133