MOLECULAR DYNAMICS STUDY OF STRUCTURE FORMATIONS IN STRONGLY COUPLED PLASMA

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Molecular Dynamics Study of Structure Formations in Strongly Coupled Plasma

by

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Department of Physics

Submitted

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

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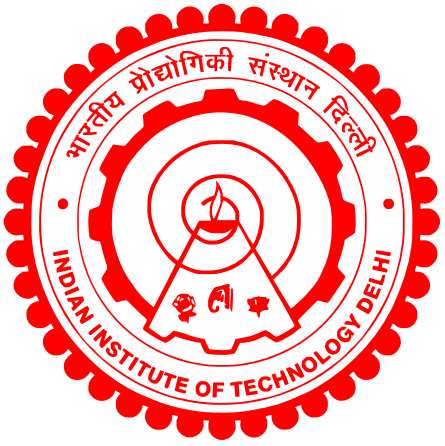

INDIAN INSTITUTE OF TECHNOLOGY DELHI

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Dedicated to my family and friends

Certificate

This is to certify that the thesis entitled **"Molecular Dynamics Study of Structure Formations in Strongly Coupled Plasma "**, submitted by **Mamta** to the Indian Institute of Technology Delhi, for the award of the degree of **Doctor of Philosophy** in PHYSICS, is a record of the original, bona fide research work carried out by her under my supervision and guidance. The thesis has reached the standards fulfilling the requirements of the regulations related to the award of the degree.

The results contained in this thesis have not been submitted 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.

Prof. Amita Das
Department of Physics,
Indian Institute of Technology Delhi.

Date:

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Abstract

This thesis focuses on the study of structure formations and their dynamics in strongly coupled plasma regimes with the help of Molecular Dynamics (MD) simulations using an open-source code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator).

The work primarily concentrates on the two strongly coupled regimes of plasma physics i.e. Ultracold plasma and Dusty plasma. In ultracold plasma, the study examines the formation of classical bound structures and also understands the shielding profile in a strongly coupled regime. At equilibrium, various kinds of classical bound structures have been observed. Another aspect of this regime, i.e., the shielding profile, is understood by externally inserting a highly charged particle, which mimics a probe in experiments. The crystalline structures have been observed around this externally inserted particle in two- and three-dimensional simulations. The potential profile of the shielding cloud has been compared with the Debye shielding profile. Also, the dynamics of the shielding cloud have been observed under the influence of external forces.

In dusty plasma medium, the transition of the dynamics of dust clusters from the macroscopic to the microscopic regime passing through the mesoscopic regimes has been studied. These regimes are classified depending on the ratio of particles on the surface to the bulk in the dust cluster, similar to that observed in the condensed matter. The emergence of an extra ring with the addition of particles, is always preceded by structures exhibiting pentagonal symmetry in the core. The dependence of the formation of pentagonal structures under various symmetry of boundary conditions (square, hexagonal, and pentagonal) has been studied in detail.

सार

यह शोधप्रबंध दृढ़ युग्मित प्लाज़्मा में संरचना निर्माण तथा उनकी गतिकी के अध्ययन पर केंद्रित है। इस अध्ययन में आणविक गतिकी अनुकरण की सहायता ली गई है, जिसके लिए मुक्त स्रोत संहिता **LAMMPS** (विशाल-पैमाने परमाण्विक/आणविक बहुल-समन्वित अनुकरणकर्ता) का उपयोग किया गया है।

यह कार्य मुख्यतः प्लाज़्मा भौतिकी के दो दृढ़ युग्मित क्षेत्रों – अर्थात् अत्यंत शीतल प्लाज़्मा और धूलिकणीय प्लाज़्मा – पर केंद्रित है। अत्यंत शीतल प्लाज़्मा के अध्ययन में पारंपरिक बंधित संरचनाओं के निर्माण की जांच की गई है तथा दृढ़ युग्मित अवस्था में आवरण की रूपरेखा को समझने का प्रयास किया गया है। संतुलन की अवस्था में विभिन्न प्रकार की पारंपरिक बंधित संरचनाएँ देखी गई हैं। इस क्षेत्र का एक अन्य पहलू, अर्थात् आवरण की रूपरेखा, को समझने के लिए बाहरी रूप से एक अत्यधिक आवेशित कण डाला गया है, जो प्रयोगों में प्रयुक्त जांच कण की तरह कार्य करता है। इस बाहरी रूप से डाले गए कण के चारों ओर द्वि-आयामी तथा त्रि-आयामी अनुकरणों में स्फटिकीय संरचनाएँ देखी गई हैं। आवरण मेघ की विभव रूपरेखा की तुलना डेबाई आवरण की रूपरेखा से की गई है। साथ ही, बाहरी बलों के प्रभाव में आवरण मेघ की गतिकी का भी अवलोकन किया गया है।

धूलिकणीय प्लाज़्मा माध्यम में, धूलिकण समूहों की गतिकी का संक्रमण मध्यवर्ती स्तर से होते हुए स्थूल स्तर से सूक्ष्म स्तर की ओर परिवर्तन का अध्ययन किया गया है। इन स्तरों का वर्गीकरण धूलिकण समूह में सतह पर स्थित कणों और आंतरिक कणों के अनुपात पर निर्भर करता है, जो कि संघनित पदार्थ में देखे गए व्यवहार के समान है। पंचभुजीय सममिति वाली संरचनाएँ हमेशा केंद्र में प्रकट होती हैं जब भी कणों के जुड़ने के साथ एक अतिरिक्त वलय उत्पन्न होता है। सीमा स्थितियों (वर्गाकार, षट्भुजाकार, तथा पंचभुजाकार) की विभिन्न सममितियों के अंतर्गत पंचभुजीय संरचनाओं के निर्माण की निर्भरता का विस्तृत अध्ययन किया गया है।

Contents

List of Figures

List of Tables