ABSTRACT

of the dissertation for the degree of Doctor Philosophy
Specialty "6D070500 - Mathematical and computer modeling"

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COMPUTER SIMULATION OF DUSTY PLASMA IN AN EXTERNAL MAGNETIC FIELD

In the present dissertation work the computer simulation of an ensemble of charged particles were performed on the basis of the molecular and langevin dynamics computer simulation method, with taking into account the external uniform magnetic field. For this purpose mathematical models of dusty plasma and processes in it were built, a numerical scheme for integrating the equations of motion was obtained, taking into account the influence of an external magnetic field and friction force, where the time step does not depend on the magnitude of the magnetic field.

Relevance of the dissertation theme. The dissertation uses computer simulation based on the methods of molecular and langevin dynamics. The molecular dynamics method is one of the powerful computational methods based on the numerical solving the classical equations of particles motion in a certain volume of the environment, and is effectively used to simulate the physical and biological systems and allows to consider the time evolution of a system consisting of large number of particles.

The investigation of the behavior and properties of an ensemble of charged particles using the computer simulation methods is of great interest in scientific world in the last decades. Special attention is paid to the case when the system is strongly coupled, i.e. when the Coulomb interaction of particles exceeds their kinetic energy. Dusty plasma is a notable type of strongly coupled many particle system. Such systems are often found in astrophysical environments, and can also be realized in laboratory conditions. Dust particles are micron-sized particles of condensed matter that can be formed in plasma reactors as a result of sputtering of wall material, chemical reactions and agglomeration processes, or entering the plasma from the outside. The dust particles with relatively large surface area, when enter the plasma, are charged with fluxes of plasma electrons and ions up to very large values of the electric charge. Under terrestrial conditions, the charge is most often negative due to the greater mobility of the electrons. A large charge causes a strong electrostatic interaction of dust particles with each other and affects the properties of the dusty plasma, in some cases leading to the appearance of ordered structures, so-called plasma crystal. Dusty plasma, which is formed, in particular, in the near-wall region of controlled thermonuclear fusion (CTF) installations with magnetic confinement, is strongly coupled magnetoactive plasma. Wall dusty plasma seriously affects to the flow of the processes in the installations of the TCB. In particular, the diffusion coefficient is associated with plasma confinement in magnetic traps, with energy

losses of slow radiation in dense plasma, which is particular interest for inertial thermonuclear fusion installations, as well as installations with heating from ion beams. Also, dusty plasma is a useful tool for studying many physical processes occurring in a many particle systems.

Prospects for the use of dusty plasma and plasma crystals in nanotechnology, computer and other technologies are widely discussed. Thus, dust and buffer plasma form a very interesting object - dusty (complex) plasma, which has unique properties and behavior, which is the reason for choosing such a system for computer simulation.

A review of the scientific literature and analysis of the development of models and methods in the field of mathematical simulation shows that in recent decades a significant amount of work has been done on the study of the properties of many particle systems using computer simulation methods. However, most of these works do not take into account the dissipation in the system, which is associated with the presence of background plasma, or are performed for unmagnetized case. The tasks of this dissertation work include the development of mathematical models for describing processes in dusty plasma with taking into account the Lorentz force and the dissipative term in the equations of motion of dust particles, creating a software package to study the effect of dissipation and a magnetic field on the properties of a strongly coupled dusty plasma.

The purpose of the dissertation.

The main goal of this dissertation work is to develop computer programs for modeling the processes in a magnetized dusty plasma using molecular and langevin dynamics, taking into account the dissipation (friction forces) in the system, applying the computer simulation results to study and analyzing of the dynamic, structural, and transport properties of dusty plasma.

The object of research is a magnetoactive dusty plasma.

The subject of research is mathematical models and numerical schemes necessary for computer simulation of the physical properties of dusty plasma, as well as the results of the simulation itself.

To achieve this goal it was necessary to solve the following tasks:

– to build a mathematical model for computer simulation of magnetically active dusty plasma;

– to carry out computer simulation of magnetically active dusty plasma, which allows the correct study of the properties of dusty plasma;

– to create a mathematical model for directional correlation functions that adequately describe the processes of particle localization along and across the direction of an external magnetic field;

– to build an automated complex of computer programs for modeling and studying the properties of dusty plasma.

The main provisions for the defense:

– The constructed mathematical model for computer simulation of magnetically active dusty plasma allows one to correctly take into account the influence of an external magnetic field and friction force on the dynamics of dust particles in a buffer plasma;

– Performed computer simulation allows to correctly investigate the structural (pair correlation function) and dynamical (autocorrelation function of velocities and diffusion) properties of dusty plasma.

– The constructed mathematical model for directional correlation functions adequately describes the processes of localization of particles along and across the external magnetic field;

– An automated complex of computer programs for modeling and investigation of the properties of dusty plasma was built.

Scientific novelty of the dissertation results.

The scientific novelty and originality of the dissertation work lies in the fact that for the first time in it:

– Numerical scheme which takes into account the effects of an external magnetic field and friction force was obtained, where the time step does not depend on the magnitude of the magnetic field;

– Computer simulations, allowing to correctly investigate the properties of dusty plasma were performed;

– Mathematical model for directional correlation functions, which adequately describe the processes of localization of particles along and across the direction of the external magnetic field was constructed;

– Automated complex of computer programs for modeling and studying the properties of dusty plasma was built.

Practical importance of the dissertation.

The practical significance of the research is dictated, in particular, by the vital necessity of the development of the energy sector, which uses a practically unlimited resource, safe in operation and sufficiently pure in ecological terms. In this regard, in recent decades, major projects have been developed (for example, ITER, NIF, etc.) related to the development of thermonuclear power engineering. In the course of work on the creation of thermonuclear installations with magnetic confinement, it was noticed that in the near-wall region of the discharge chambers a large amount of dust is generated, which significantly affects the processes occurring in the central region. Thus, the construction of mathematical models for modeling and research of dynamic, transport and other properties of dusty magnetoactive plasma is a great importance, both on a national and international scale.

Validity and reliability of the results.

The mathematical model is based on the use of the classical molecular dynamics (MD) and Langevin dynamics methods which takes into account the dissipation in the system (friction force), as well as specially selected equations for processing data

from a computer experiment. To integrate the equations of motion of particles, a reliable Verlet algorithm was used, based on the expansion of the velocity and coordinates of particles in a Taylor series. The constructed mathematical model also includes equations for cage correlation functions, which are written firstly in the dissertation for components parallel and perpendicular to the external magnetic field. The results on diffusion and cage corelation functions are in a good agreement with the data of physical experiments and the results of other authors.

Validity and reliability of the results are confirmed by publications in foreign journals with a high impact factor and in publications recommended by the Committee on the Control of Education and Science of the MES RK, and in the works of international scientific conferences in the near and far abroad.

The personal contribution of the author. The author fulfilled the research, solved the problems and made numerical calculations. Formulation of the problems, choosing the method of investigation and discussion of the results were carried out together with scientific supervisors.

Publications. According to the materials of the dissertation, 42 publications were published: 11 in journals from the List of KKSON MES RK for publication of the main results of the thesis for the PhD degree and 8 articles in foreign journals with impact factor included in the international information resource Web of Knowledge (Thomson Reuters , USA) and Scopus (Elsevier, the Netherlands); 21 papers in materials of the International Scientific Conferences and 2 copyright testimony.

Approbation of the dissertation. The results obtained in the thesis were reported and discussed:

–at the International Conference of Students and Young Scientists «Mir nauki» (2013, 2014, Almaty, Kazakhstan);

–at the 51 – st International Conference «Student and technological progress» (2013, Novosibirsk, Russia)

- At the International Scientific Conference dedicated to the 75th anniversary of Academician of NAS RK Abildin Meirkhan Mubarakovich “Actual problems of modern physics” (2013, Almaty, Kazakhstan);

–at the International Conference «The International Conference on Phenomena in Ionized Gases (IIGPIG)» (2015, Iasi, Romania);

–at the International Conference«International Conference on the Physics of Dusty Plasmas (ICPDP - 7)» (2014, New Delhi, India)

–at the International Conference«15th International Conference on the Physics of Non-Ideal Plasmas (PNP)» (2015, Almaty, Kazakhstan);

–at the International Conference «21st International Symposium of Heavy- Ion Inertial Fusion (HIF)» (2016, Astana, Kazakhstan);

–at the International Conference«XXII Europhysics Conference on Atomic and Molecular Physics of Ionized Gases (ESCAMPIG)» (2016, Bratislava, Slovakia);

–at the International Conference«International Conference on Strongly Coupled Coulomb Systems (SCCS)» (2017, Kiel, Germany);

–at the International Conference«The International Conference on Research and Application of Plasmas (PLASMA)» (2017, Warsaw, Poland);

–at the International Conference«42nd European Physical Society Conference on Plasma Physics (EPS)» (2018, Prague, Czech Republic);

–at the International Conference«XV Russian conference (with international participation) on thermophysical properties of substances (RCTP-15)» (2018, Moscow, Russia);

–at the International Conference «Modern advances in physics and fundamental physical education» (2016, Almaty, Kazakhstan);

–at the International Conference of Students and Young Scientists «Farabi alemi» (2015, 2016, 2017, Almaty, Kazakhstan);

–at the International Conference «XXIX IUPAP Conference on Computational Physics (CCP2017)» (2017, Paris, France);

–at the International Conference «SDFFO-9» (2016, Almaty, Kazakhstan);

–at the 10th International Scientific Conference «Chaos and Structures in Nonlinear Systems. Theory and Experiment» dedicated to the 75th anniversary of Professor Z.Zh Zhanabayev" (2017, Almaty, Kazakhstan);

- at scientific seminars of the Department of Plasma Physics and Computer Physics of the Kazakh National University. al-Farabi;

- at scientific seminars of the Institute of Information and Computing Technologies of the Ministry of Education and Science of the Republic of Kazakhstan.

Relation of the dissertation theme to the plans of scientific research. The dissertation work was fulfilled in accordance with the plans of the following fundamental scientific research works (SRW) SC RK MES "Grant funding for scientific research" on the topics:

– «Elementary processes and optical properties of plasma with a complex composition of inertial thermonuclear fusion» (2015-2017 yy., registration № 0115PK01037, 3102/GF4);

– «Computer simulation of the properties of magnetoactive plasma of complex composition» (2015-2017 yy., registration №0115PK01037, 3087/GF4);

– «The study of dust-sound solitons in a magnetically active plasma of complex composition» (2018-2020 yy., registration №0118PK00609, AP05132665/GF);

– Targeted financing programs «Investigation of the fundamental problems of plasma physics and plasma-like media» (2018-2020 yy., BR05236730/GF);

– «Development and research of mathematical models, numerical methods and a complex of combinatorial optimization programs (for example, rectangular cutting problems)» (2015-2017 yy.);

– «Research and development of models and methods for presenting and organizing knowledge using the ontological approach and Smart technology tools when implementing educational programs and processes» (2018-2020 yy., registration №AP05134973);

– «The development of information technologies and systems to stimulate the

sustainable development of the individual as one of the foundations for the development of digital Kazakhstan» (2018-2020 yy., BR05236839/GF).

The volume and structure of the dissertation. The dissertation work consists of an introduction, 4 chapters, conclusion and the list of references from 154 titles, contains 135 pages of basic computer text including 73 figures and appendices.