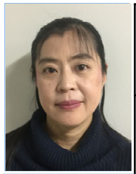
【Grant-in-Aid for Transformative Research Areas（A）】

Quantum Matter Science in the Universe Opened Up by Precise Numerical Calculations



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Project Information	Project Number : 25A203	Project Period (FY) : 2025-2029
	Keywords : Finite quantum many-body systems, precise numerical calculations, high density nuclear matter, interstellar molecules, heavy element synthesis	

Purpose and Background of the Research

●Outline of the Research

A major research goal in physics is to elucidate the formation and evolution of matter in the universe as shown in Figure 1. In the process of material evolution in space, there are various issues that need to be resolved. How did molecules form in space? How were heavy elements such as uranium formed? What kind of particles form the interior of neutron stars, the final form of material evolution?

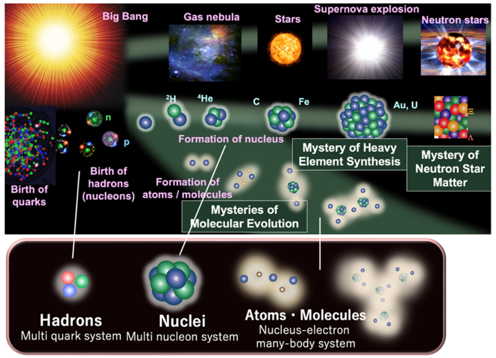

Figure 1. Illustration of the evolution of matter in space

These issues will be solved at once if the fundamental equations (Schrödinger equation) of finite quantum many-body systems (up to about 100) interacting by electromagnetic and nuclear forces can be solved with high precision. However, as the number of particles increases, the computational resources become enormous, so calculations based on theoretical models that capture the characteristics of the system have been used instead of precise calculations. Since the parameters in the model are determined to reproduce the existing experimental data, the current calculation method is unreliable and is difficult to interpretate highly precise experimental data . Moreover, the lack of predictive power for objects for which no experimental data exist is a major problem.

Therefore, we aim to establish a high-precision calculation method for finite quantum many-body systems that can be applied across a wide range of hierarchies, from atoms and molecules to nuclei and hadrons. As shown in Figure 2, we will integrate and unify the Gaussian expansion method (GEM), which is an exact calculation method applicable to particle systems of up to 10 particles, and the large-scale shell model (LSM) and density functional theory (DFT). The unified calculation platform will be constructed to handle quantum many-body systems with the number of particles ranging from 3 to 100 with high precision. By combining this unified platform with experimental studies at each hierarchy, we will try to elucidate the structure of neutron star interiors, the evolutionary process of interstellar molecules, and the synthesis process of heavy elements.

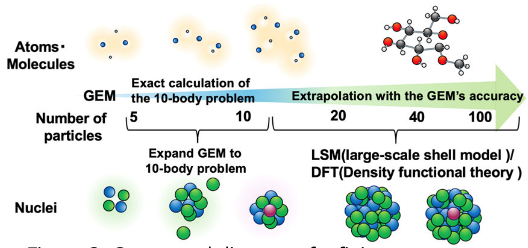

Figure 2. Conceptual diagram of a finite quantum many-body system computing platform based on GEM

Figure 3 shows the overall picture of this area. The numerical theory group (A01, 02, 03) is placed at the center of this area and aims to establish a unified platform for finite quantum many-body system computations. Together with experimental group (B01, B02, B03, B04), we aim to elucidate the evolutionary formation of quantum matter in the universe.

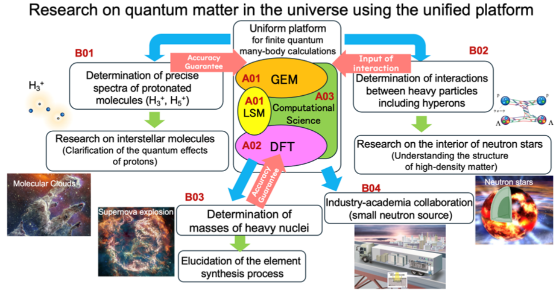

Figure 3. Overview of this field

Expected Research Achievements

●Transformation brought about by the unified platform (A01, 02, 03)

Computational science has made significant progress with the appearance and operation of the world's fastest supercomputer “Fugaku”. By collaborating with experts in computational science, precise computation of quantum many-body systems has become a reality. We will build a unified platform for finite quantum many-body calculations that integrates and unifies GEM, LSM, and DFT. This will revolutionize the fields of nuclear physics, quantum chemistry, and related field, as well.

● Interstellar molecular research transformed by nuclear quantum effects (B01)

H_3^+ and H_5^+, called protonated molecules, are present in interstellar molecular clouds and, due to their high reactivity, are the starting point for the formation of more complex molecules such as water and hydrocarbons. In order to elucidate the formation mechanism of these interstellar molecules, it is important to perform calculations that explicitly incorporate the quantum effects of intramolecular protons. In this field, we aim to elucidate interstellar molecular evolution by comparing high-precision calculations of H_3^+ and H_5^+ that incorporate quantum effects of proton nuclei with experiments.

●Towards elucidating the inner structure of neutron stars (B02)

To understand the internal structure of neutron stars, it is essential to understand the interaction between heavy particles containing strange quarks called hyperons. We aim to elucidate the neutron internal structure by conducting joint research with experiments and theories to determine the interactions between them, and also by performing precise calculations of nuclei containing hyperons (hypernuclei).

●Unraveling the synthesis of heavy elements in the universe (B03)

In the experiment at RIBF, we plan to measure the masses of rare-earth nuclei with high precision. We will compare the experimental values and theoretical calculation by the unified platform to guarantee the accuracy of the DFT calculation. After the completion of this field, we aim to construct a DFT that can predict the masses of nuclei in regions that cannot be reached through experiments cannot. The ultimate goal is to elucidate the synthesis of heavy elements in the universe through numerical experiments.

●Impact on industry-academia collaboration (B04)

This area can also contribute to small neutron sources that can be used for nondestructive testing of bridges and other social infrastructure. By determining the neutron spectrum when ^9Be or ^7Li is irradiated with low-energy protons and the reaction cross section between fast neutrons and materials using the unified platform with high precision, we will support RIKEN's development of a small neutron source, RANS.

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