

A Python package for the commutator of many-body operators

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Abstract

In recent years, the In-Medium Similarity Renormalization Group (IMSRG) has been making great progress in ab initio nuclear many-body theory. At present, the many-body operator is generally truncated to two-body in the IMSRG. In order to extend the many-body truncation to the normal-ordered three-body level, it's necessary to develop the IM-SRG(3), which involves a great number of complex calculation processes of many-body operators. Therefore, writing a computer program to achieve auto-calculation would help researchers reduce the cost of time and energy on such processes.

To achieve the program, it is necessary to translate the theoretical calculation process into a series of algorithms and apply these algorithms to the calculation of symbols. Under the Python platform, based on the computer algebra system provided by SymPy, this Python package, called combo, can create objects of related classes to indicate the indicators and operators. By applying these objects to a series of algorithms, the combo can calculate the commutator of two arbitrary many-body operators. Moreover, after solving the problem above, an interface function matching the Angular Momentum Coupling Program (AMC) is written and can give the result that coupled the angular momentum.

Specifically, four modules in this package can: a) calculate the product and commutator of two arbitrary many-body operators, b) apply symbols' rule c) regulate the expressions and provide some auxiliary functions. d) process the expressions for output.

Based on the functions above, the combo package not only can reproduce the relevant calculational process in the IMSRG but also lays the foundation for the development of IMSRG(3). This paper introduces the function of each module of this package and illustrates the algorithm's workflow in some logic diagrams.

Keywords: Python, IMSRG, commutator of normal-ordered operators, combo

Program summary

Program Title: combo

CPC Library link to program files:

Developer's repository link: <https://github.com/liviler/combo>

Code Ocean capsule:

Licensing provisions: GPLv3

Programming language: Python 3.10

External routines: sympy

Nature of problem: The IMSRG achieves success in nuclear physics research. However, the works to calculate the commutator of normal-ordered operators is error-prone and would cost a lot of time. And the length of result will grow rapidly as a factorial function.

Solution method: To calculate the product and commutator of normal-ordered operators, combo uses Wick's theorem to match all possible indicators combinations with the operators and ignore the inappropriate combinations. Afterwards, combo can split the previous expression and regulate it. And you can display all attributes that store the result of your behaviour. Moreover, an interface function is given to match the Angular Momentum Coupling Program (AMC).

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1. Introduction

2. Theoretical background

3. Implementation

3.1. Algorithm

3.2. Code structure

3.3. Usage

4. Conclusion and outlook

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References