A Simple Method of Calculating Commutators in Hamilton System with Mathematica Software

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Abstract

As a powerful tool in scientific computation, Mathematica offers us algebraic computation, but it does not provide functions to directly calculate commutators in quantum mechanics. Different from present software packets to deal with noncommutative algebra, such as NCAlgebra and NCComAlgebra, one simple method of calculating the commutator in quantum mechanics is put forward and is demonstrated by an example calculating SO(4) dynamical symmetry in 3 dimensions Coulomb potential. This method does not need to develop software packets but rather to directly write program in Mathematica. It is based on the connection between commutator in quantum mechanics and Poisson bracket in classical mechanics to perform calculations. Both the length and the running time of this example are very short, which demonstrates that this method is simple and effective in scientific research. Moreover, this method is used to calculate any commutator in Hamilton system in principle. In the end some deficiencies and applications are discussed.

Key words: Commutator, Noncommutative Algebra, Poisson Bracket

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1 INTRODUCTION

Today scientific computations are classified into two kinds. One is pure numerical computation, the other is algebraic computation. The latter treats with symbolic computation rather than simple numerical computation, thus it holds more general applications in scientific research. Among much software

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to implement symbolic computation, Mathematica, developed by Wolfram Research Inc., is one of the most popular, influential and active software in academic and industrial world [1]. It offers us powerful scientific computational facilities, algebraic computation, high-quality graphical visualization and user interfaces. Moreover, its basic system is developed in C program language, and it is easy to be transplanted into other programs and languages.

Mathematica has been extensively applied in scientific research, especially in mathematics, physics and chemistry. For instance, it has been used to solve Schrödinger equation for bound states [2], calculate tree-level multi-particle electroweak production process [3], and perform numeric computation of dyadic Green’s function [4]. But there still exist many other problems on symbolic computations to be simplified. Calculating commutators in quantum mechanics is one of such problems.

The emergence of the commutator is a fantastic event in physics [5]. In classical mechanics there does not exist noncommutative quantity, while in quantum mechanics, there are two kinds of quantities: Q quantity and C quantity. Q quantity denotes noncommutative quantity. For example, when two quantities $A, B$ do not meet commutative law, i.e. $[A, B] = AB - BA \neq 0$, we may say that $A, B$ are two Q quantities. Otherwise, we may say that $A, B$ are two C quantities. In quantum theory, especially in quantum mechanics, quantum group and statistical physics, we often have to calculate many commutators.

Today the research of the commutator has initiated noncommutative algebra [6] and noncommutative geometry [7,8], which are all hot topics in physics.

However, in practice, to perform these symbolic calculations is a tedious and mechanical job for physicists, so it is necessary to seek a simple and effective method of calculating operators with computer. It should be noted that even though Mathematica does provide symbolic computations, it does not include calculating commutators yet. Therefore, a direct idea is to develop source codes in Mathematica to compute commutator or anti-commutator. Along this routine, scientists have developed some software packets to deal with noncommutative algebra [9–11], such as NCAIgebra [9] and NCComAlgebra [10], to perform symbolic computations. On one hand, to develop, install and use these professional packets need many skills and knowledge of computer, which might be hard work for most physicists. On the other hand, in these packets, we should set the basic commutative relations firstly, and then by using computer, we simplify these operators. The process makes it inconvenient to calculate commutator with this software. Moreover, some software is commercial and it would not be used free. Hence, if one simple way to calculate the commutator is put forward, it will bring us convenience in practical research. After all, we need a simple method. Actually, noted that Mathematica provides differential calculation, and with the relation between commutator in quantum mechanics and Poisson bracket in classical mechanics, it might be
used to calculate the commutators. Based on this idea, one simple, easy new method of calculating commutators in Hamilton system is presented and its process is illustrated by one example in this article. The method does not need to develop any software packet or modify any source code in Mathematica and it executes calculations only with functions in Mathematica software itself. It should be noted that this method is very simple and it does not need other extra skills or knowledge of computer. Moreover, this method can be extended into solving more problems. In the end some defects and applications of this method are discussed. This method is expected to simplify many practical computations in further scientific research.

2 POISSON BRACKETS AND COMMUTATORS

Now let us recall the relation between Poisson bracket and commutator

\[ \{A, B\} = \frac{1}{i\hbar} [A, B], \] (1)

where \([\ ]\) donates commutator, \(\{\}\) donates Poisson bracket\([12]\), \(i\) is the imaginary number unit, and \(\hbar\) is Planck’s constant. This relation gives us the connection between the quantum mechanics and classical mechanics. Assume a Hamilton system \(H(p_i, q_i)\), where \(p_i, q_i\) are canonical coordinates and their conjugate momenta respectively. For two mechanical quantities \(A(p_i, q_i), B(p_i, q_i)\), the Poisson bracket is defined by \([13]\]

\[ \{A, B\} = \sum_i \left( \frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right). \] (2)

From Eq.(1) and (2), we will obtain

\[ [A, B] = i\hbar \sum_i \left( \frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right). \] (3)

Eq.(3) provides some clues to calculate commutators. It should be noted that the left side of eq.(3) is noncommutative algebra, but the right-hand side becomes a polynomial in classical mechanics and there does not exist noncommutative algebra. i.e. eq.(3) give us a tool to change noncommutative algebra calculations into commutative algebra calculations. When we compute commutators in quantum mechanics, we firstly rewrite these commutators into Poisson brackets in classical mechanics. Then we could use the functions in Mathematica directly to calculate those Poisson brackets, and at last we rewrite the results into quantum operators and get calculating results. Because
Mathematica provides powerful functions, such as Factor, Simplify, D[f,x] [1], we can effectively finish complex calculations in a few minutes. In the next section we will describe this method by computing SO(4) group in 3 dimensions Coulomb potential.

3 CALCULATING SO(4) GROUP IN 3 DIMENSIONS COULOMB POTENTIAL WITH MATHEMATICA

Assume a particle in Coulomb potential \( V(r) = \frac{-1}{r} \), we try to calculate the dynamical symmetry group SO(4). In 3 dimensions Coulomb potential, there exist three conserved quantities, Hamiltonian \( H \), angular momentum \( L \) and Runge-Lenz vector \( R = \frac{1}{2}(P \times L - L \times P) - e_r \) [14]. In order to know whether angular momentum \( L \) and Runge-Lenz \( R \) construct SO(4) Lie group, we should calculate the commutators \([H, R], [R, R], [R, L], [L, L]\). Firstly we calculate the commutator \([R, R]\). In fact from the symmetry, we might only calculate the commutator \([R_x, R_y]\), where \( R_x, R_y \) are Runge-Lenz vector \( R \) along \( x \) and \( y \) axis respectively. Generally, calculating these commutators is a tedious job, but we will show that with Mathematica it becomes a piece of cake.

First. Simplify the commutator to be calculated with the algebra relation \( P \times L + L \times P = 2i\hbar P \). Then, we obtain

\[
[R_x, R_y] = \frac{1}{2}(P \times L - L \times P) - e_r.
\]

In most circumstances, we should simplify the commutators before we calculate these commutators.

Second. Using eq.(1) and eq.(4), we rewrite above commutator into Poisson bracket as follows:

\[
[R_x, R_y] = i\hbar \{(P \times L - i\hbar P)x - e_x, (P \times L - i\hbar P)y - e_y\}.
\]

here we should note the definitions \((P \times L)_x = i\hbar(l_z p_y - l_y p_z), l_x = i\hbar(y p_z - z p_y)\)
and \( e_x = \frac{x}{(x^2 + y^2 + z^2)^{\frac{3}{2}}} \), \( e_y = \frac{y}{(x^2 + y^2 + z^2)^{\frac{3}{2}}} \) etc.

Third, eq.(5) also can be rewritten into

\[
[R_x, R_y] = i\hbar \sum_{i,p} \left( \frac{\partial}{\partial i}((P \times L - i\hbar P)x - e_x) \frac{\partial}{\partial p_i}((P \times L - i\hbar P)y - e_y) \right. \\
- \left. \frac{\partial}{\partial p_i}((P \times L - i\hbar P)x - e_x) \frac{\partial}{\partial i}((P \times L - i\hbar P)y - e_y) \right)
\]
where $i = x, y, z$; $p_i = p_x, p_y, p_z$. Using the function in Mathematica (see Appendix), we could directly calculate the right-hand of eq. (6) as follows

$$[R_x, R_y] = -i\hbar(p_y x - p_x y)(P^2 - \frac{2}{r}).$$

(7)

Similarly, we could calculate other commutators with Mathematica.

$$[H, R_x] = 0,$$

(8)

$$[L_x, R_y] = -i\hbar(p_x p_z x + p_y p_z y - z p_x^2 - z p_y^2 - i\hbar p_z - \frac{z}{r}),$$

(9)

$$[L_x, L_y] = -i\hbar(x p_y - y p_x).$$

(10)

Fourth, rewrite above results into the standard quantum mechanics operators and simplify these results. We get

$$[R_x, R_y] = -2i\hbar HL_z,$$

(11)

$$[H, R] = 0,$$

(12)

$$[L_x, R_y] = i\hbar R_z,$$

(13)

$$[L_x, L_y] = i\hbar L_z.$$

(14)

Up to now we have finished calculating such tedious commutators. From above relations, we can see that the Rungle-Lenz vector $R$ and angular momentum $L$ construct the SO(4) dynamical symmetry, which is higher than geometry symmetry SO(3). This is a well-known result in quantum mechanics [15,16]. What we want to do here is not to prove or check this result, but to demonstrate that our method is efficient. It should be noted that the program is very short (only 20 lines) and the running time is only half a minute (PC 300, 64MB RAM)! In contrast to calculating above commutators by hand, it is faster and more exact. The program and some expeditions are listed in Appendix and there the function Commutator3D can be used to compute any commutator in 3 dimensions Hamilton system.

4 DISCUSSIONS

Because the connection between the commutator and Poisson bracket only helps to calculate the Hamilton system in quantum mechanics, our method might be unsuitable for the second quantize system. However, it does provide a simple and powerful method of calculating or checking commutators
on dynamics symmetry and Lie algebra in quantum mechanics and classical mechanics, especially when the Hamiltonian contains complicated potentials. In principle, this method is used to calculate any commutator in Hamilton system. We test our method in several problems, such as calculating Lie algebra or Lie group in isotropic harmonic potential [17], screened Coulomb potential and screened isotropic harmonic potential [18]. All of the results have demonstrated that this method is simple, effective and robust. We expect this method could help physicists solve such problems easily. Moreover, this method is easy to be applied into other mathematical software, such as Maple, Matlab. Meanwhile our method indeed shows that for calculating most commutators in Hamilton system, Mathematica could solve these problems by itself.

Of course, it is interesting and valuable to develop these software packets [9–11] to perform symbolic calculations, because they will release us from the bondage of mechanical and tedious work, and help us conduct real scientific research. In contrast to using these software, our method seems to be simpler and easier for most physicists. Of course, this method could not take the place of these software packets and itself is only supplement to these software packets. Actually we also hope that our method could give some clues in developing noncommutative algebra software and make it more powerful.

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APPENDIX

(*This program is used to calculate the SO(4) group in 3D Coulomb potential \( V(r) = -1/r \) *)
(* Commuator3D is a function to calculate commutators in 3 dimensions, where f and g are variables to be computed *)
(* p_i and q_i (i=1,2,3) are canonical coordinates and their conjugate momenta respectively *)
(*ham is Hamiltonian of system, h is Planck’s constant, l is angular momentum and r is Rungz-Lenz vector*)

\[
\text{Commutator3D}[f_\cdot, g_\cdot] := i \ h \ \{ D[f, q_1] \ D[g, p_1] - D[f, p_1] \ D[g, q_1] + D[f, q_2] \ D[g, p_2] - D[f, p_2] \ D[g, q_2] + D[f, q_3] \ D[g, p_3] - D[f, p_3] \ D[g, q_3] \ \}
\]

\[
\text{ham} = \{(p_1^2 + p_2^2 + p_3^2)/2\} - 1/\sqrt{q_1^2 + q_2^2 + q_3^2})
\]
\begin{align*}
l_1 &= q_2 p_3 - q_3 p_2 \\
l_2 &= q_3 p_1 - q_1 p_3 \\
l_3 &= q_1 p_2 - q_2 p_1 \\
\end{align*}

\begin{align*}
r_1 &= l_3 p_2 - l_2 p_3 - i \ h \ p_1 - q_1 / \sqrt{q_1^2 + q_2^2 + q_3^2} \\
r_2 &= l_1 p_3 - l_3 p_1 - i \ h \ p_2 - q_2 / \sqrt{q_1^2 + q_2^2 + q_3^2} \\
r_3 &= l_2 p_1 - l_1 p_2 - i \ h \ p_3 - q_3 / \sqrt{q_1^2 + q_2^2 + q_3^2} \\
\end{align*}

\begin{align*}
s_1 &= \text{Commutator3D}[r_1, r_2] \\
s_2 &= \text{Commutator3D}[r_1, \text{ham}] \\
s_3 &= \text{Commutator3D}[l_1, r_2] \\
s_4 &= \text{Commutator3D}[l_1, l_2] \\
f_1 &= \text{Simply}[s_1] \\
f_2 &= \text{Simply}[s_2] \\
f_3 &= \text{Simply}[s_3] \\
f_4 &= \text{Simply}[s_4] \\
\end{align*}

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