Separation of procedures in numerics

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The present paper explains the importance of the concept of separation of procedures in numerical calculations of cooperative phenomena. A typical example of applications of this concept is to derive and to make use of exponential product formulas. Recently systematic higher-order exponential product formulas have been developed by the present author. Many applications of these higher-order formulas to physics have been reported. This study of exponential product formulas has lead to the general formulation of quantum analysis. One of the most important applications of the above exponential product formulas was given in quantum Monte Carlo methods.

Introduction

One of the basic guiding principles in theoretical sciences is the concept of separation of procedures.[1] The present author has developed many formulas and schemes of numerical calculations using this concept. One of such schemes is the Trotter-like formula.[2–5] This yields the equivalence theorem[6] between a d-dimensional quantum system and the corresponding $(d+1)$-dimensional classical system. This is the fundamental proposition for the quantum Monte Carlo method proposed by the present author.[6,7]

Quantum Monte Carlo method and negative sign problem

The main idea is to make use of the above equivalence theorem.[6] The remaining large problem of the quantum Monte Carlo method is that the so-called "negative sign problem" appears in frustrated quantum spin systems and higher-dimensional $(d \geq 2)$ Fermi systems.[8] Many authors are now trying to solve this problem by finding a clever choice of mapping and representation.[5,8–13] A more general argument will be given elsewhere.[14]

Higher-order product formulas

Recently the present author discovered a general theory of constructing higher-order exponential product formulas up to infinite order.[15–29] There have been already reported several hundred papers in which the above higher-order exponential product formulas have been used effectively. It should be emphasized that the present exponential product formulas have the great merit that they reserve symmetries of the original exponential operators such as the unitarity of the time-evolution operator and the symplectic property in nonlinear dynamics, although the Runge-Kutta method, for example, does not keep these symmetry properties.

Quantum analysis

During the above investigation of the higher-order product formulas, the present author arrived at the general formulation of quantum analysis.[30–36]

The quantum analysis is mathematics which treats non-commutative operators, in particular, quantum derivative. This is defined by the derivative of an operator-valued function $f(A)$ with respect to the operator itself A, namely $df(A)/dA$. The present author[30] introduced the same notation $df(A)/dA$ as the ordinary derivative of the c-number function $f(x)$. However the content of $df(A)/dA$ is quite different[30–36] from $df(x)/dx$. Of course, both become identical in form, when dA commutes with A.

Discussion

The present talk is hoped to stimulate new ideas in the field of computational physics.

A new scheme for treating unbounded operators, for example, a potential of Coulomb interaction will be constructed by replacing partial exponentials in the above product formulas by the Cayley formula in each step.[37]

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