

論文の内容の要旨

論文題目 Description of Fermionic Wavefunctions by Symmetric Tensor Decomposition
(対称テンソル分解によるフェルミ粒子系の波動関数の記述)

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There are a number of evidences and findings in the vicinity of quantum electronic systems in the last a few decades, such as the high T_c superconductivity in cuprates and the colossal magnetoresistance in perovskite oxides, etc. Much effort has been paid to understand these variety of challenging phenomena in condensed matter physics, but we still lack a unified and indisputable theoretical framework that can explain and predict most of these experimental facts.

The situation of the theoretical understanding for quantum many body systems has been much refreshed after the discovery of Density Matrix Renormalization Group (DMRG) method in 1992. Since then, numerical and mathematical researches in the so called tensor network frameworks have attracted considerable attention. I focus on theoretical and numerical approaches toward the tensor network framework that make use of quantum information theory and are applicable to quantum chemistry. The purpose of this thesis is to give a tensor network framework that explicitly considers the antisymmetry of the electronic wavefunction contrary to most of the previous works. With a proper consideration of the antisymmetry of the wavefunction, we can dramatically reduce the number of states constituting the total wavefunction and improve the speed of numerical calculation and enhance the convergence of the resulting energy.

In chapter 3, I introduce my recently published wavefunction theory where tensor network of the wavefunction is treated using the symmetric tensor decomposition framework with the antisymmetry of the wavefunction explicitly taken into account. This scheme is based on the configuration interaction (CI) which is a versatile wavefunction theory for interacting fermions but involving an extremely long CI series. Using a symmetric tensor decomposition (STD) method, we convert the CI series into a compact and numerically tractable form. The converted series encompasses the Hartree-Fock state in the first term and rapidly converges to the full-CI state, as numerically tested using small molecules. Provided that the length of the STD-CI series grows only moderately with the increasing complexity of the system, the new method will serve as one of the alternative variational methods to achieve full-CI with enhanced practicability.

In Chapter 4, I introduce an improvement of STD-CI. In the Extended STD (ESTD) scheme, the variational degree of freedom in the wavefunction is dramatically extended. Therefore we can expect a considerable improvement in the convergence of the energy in ESTD. And also, in ESTD we can calculate the expectation value of the energy and the first derivatives with a calculation cost proportional to N^5 , while the original scaling in STD-CI is N^6 , where N is the number of electrons. This immediately means that we can dramatically extend the size of the systems that we can treat with ESTD, compared with STD-CI. In ESTD, the wavefunction is given as a linear combination of the Antisymmetrized Geminal Powers (AGP), and the norm and energy are given through a simple formalism based on Pfaffian. We provide a comparison of numerical results of the water molecule and the Hubbard model that indicates the numerical superiority of ESTD with respect to STD-CI. Fig.1 shows a comparison of the results of the water molecule in STD and ESTD. In ESTD, the convergence of the energy with respect to the parameter K is considerably faster than STD. In future we expect to treat larger systems with ESTD, including three dimensional periodic systems. Such calculations will be propelled by the fact that in ESTD we can treat non orthogonal basis sets without taking orthonormalization, which is a procedure that significantly complicates large-scale calculations.

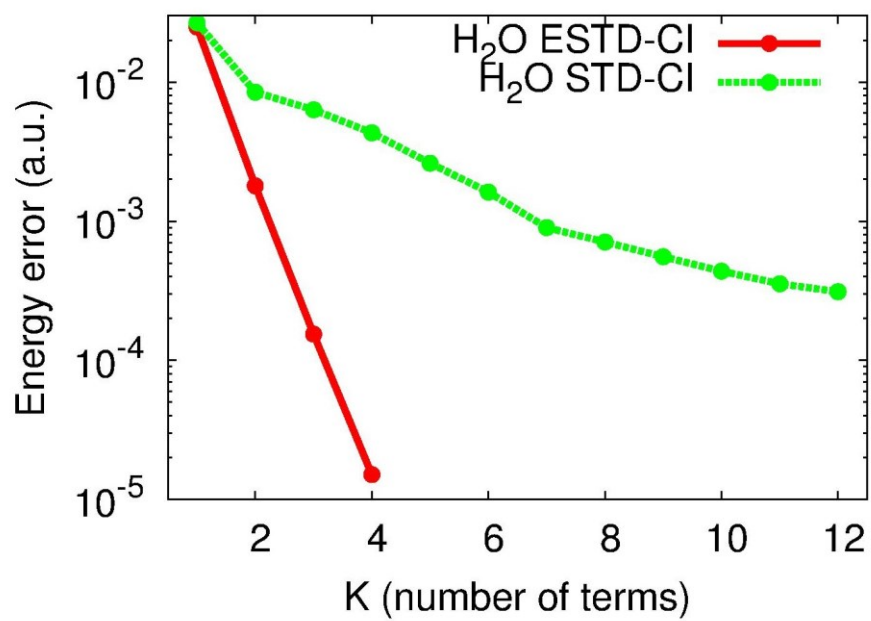


Fig.1 Comparison of the ground state energy results of the water molecule in STD and ESTD.