論文の内容の要旨

Geminal theory for strongly correlated few-body systems
(少数多体強相関系に対するジェミナル理論)

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To calculate strongly correlated systems accurately, one needs to treat strong and weak correlations simultaneously. Popular methods, such as Hartree-Fock theory or density functional theory, can treat the weak correlation but cannot treat the strong correlation. On the other hand, the full-configuration-interaction (full-CI) method can treat the strong correlation well but it needs high calculation cost. In this context, I focus on the wave function theory for the electron pair. In condensed matter physics, the electron pair is an important concept for superconductivity. Also in the field of chemistry, the concept of electron pair has been used to represent a chemical bond since a long time ago. The electron pair is called geminal in chemistry and many calculation methods using geminal were developed. The method of expressing different chemical bonds using different geminals is called antisymmetrized-product-of-geminals (APG) theory. Although the idea of APG was proposed long ago, there are few APG studies because of its high calculation cost and complexity in the calculation.

In this thesis, I overcome the computational difficulty of APG using a tensor decomposition method developed in mathematics and make the variational determination of APG tractable numerically. This makes it possible to analyze the APG wave function with- out introducing additional approximations to the geminals and thus to understand the inherent advantage and disadvantage in describing strongly correlated few-body systems. This understanding helps me to develop a method to incorporate the electron correlation beyond the original APG. This novel method is based on a polynomial extension of APG; note that the original APG has a monomial form. With the polynomial extension, I succeed in relating geminals to the valence bond even in the strong correlation regime. I

recognize the polynomial extension as an introduction of the “resonance” effect into the APG-based valence bond theory and thus is a natural improvement.
I also develop variations of the APG calculation. I develop a simplified geminal method, which is different from the ones developed previously in the literatures. I also develop a geminal method specialized for a strongly correlated impurity system embedded in a weakly correlated medium.
The present study analyzes geminal theories comparatively from (a) the simplest one, called antisymmetrized geminal powers (AGP), which is a mean-field theory of geminals, (b) APG and (c) its extension, bridging thereby the HF to full-CI via electron-pair theories of different levels. I believe that the present work has made clearer the property of geminal theory and would stimulate further sophistication of the geminal-based valence bond theory.