I would like to continue to study many-body problems of the Schrödinger equation. This field has a long history and there is a lot of accumulation of research. Nevertheless, essential difficulties have still not been solved. Considering where the difficulty comes from, I would like to tackle the problem.

As a specific problem to be solved, it is first picked up to develop methods to estimate eigenvalues and eigenfunctions of the differential operator called electronic Hamiltonian accurately with error bounds of high accuracy. Such a problem cannot be solved with meaningful accuracy by the traditional numerical analysis methods such as the finite element method mainly due to the singularity of the Coulomb potentials. The method frequently used in physics is the perturbation theory, but quantitative error estimates cannot be obtained by the perturbation theory in principle. Compared to these methods, the variational method gives a part of information of the true solution, and since the eigenvalues obtained by the variational method are greater than the true eigenvalues, upper bounds of the true eigenvalues are obtained. However, it is impossible to judge how close the upper bound is to the true eigenvalue only by the variational method. From this fact we can see that in order to estimate the eigenvalues we need to find an accurate lower bound which compensates for the upper bound and shows that the true eigenvalue is greater than some value. The lower bound of eigenvalues also has a long history and there are several methods, but there is no method which is applicable to the many-body problem and has high accuracy at present. Because of these reasons, development of a method for accurate lower bounds to eigenvalues is raised as a central subject of my future research. Compared to the fact that upper bounds can be obtained by the variational method easily in principle, currently known methods for lower bounds are complicated, the execution of the calculation in the methods is difficult or impossible, and the methods have very low accuracy. Therefore, it seems to be needed to clarify the reason why the accurate lower bounds are extremely difficult.

I would like to study also upper bounds by the variational method. The problem in the variational method is how to choose the basis functions that approximate true eigenfucntions. Currently, the basis functions mainly used to approximate the behaviors of electrons near nuclei are STO and GTO. Besides, in a region in a crystal apart from nuclei plane waves are used. However, there is no theoretical guarantee that STO or GTO gives good approximation for molecules in the variational method. In particular, in a region apart from nuclei the error from the true eigenfunction is thought to be large. Moreover, in a crystal we need to connect STOs near nuclei and the plane waves in the other region on the boundaries of the regions. From such a perspective it seems that we need to develop a variational method that uses different basis functions in different regions. Since in general it is impossible to connect basis functions exactly, a method that allows discontinuity on the boundary and gives estimates for errors due to the discontinuity is needed. I would like to develop methods to connect solutions on the boundaries of regions and the estimates of errors due to the discontinuity.

As another important direction of the research, the relation between structures of eigenfunctions of different electronic Hamiltonians is raised. For example, when two molecules are connected to construct a new molecule, the new molecule often preserves the local structures such as functional groups of the original molecules almost as they are. This means mathematically that there exists a relation between the eigenfunctions of the Hamiltonians of the original molecules and that of the connected molecule. However, the eigenfunction is a function of the coordinates of the electrons spreading around the whole molecule, and the relation between the structure of the Hamiltonian and the local structure of the eigenfunction would be very complicated, ambiguous and elusive. Therefore, it is not easy to relate local structures of eigenfunctions of different Hamiltonians mathematically. An approach that seems to be promising at present is to approximate the wave function by the Slater determinant and approximate further each electronic orbital by a linear combination of a finite basis set to reduce the problem to that of finite-dimensional vectors interacting under the Hartree-Fock framework. I am planning to prove the preservation of electronic structures considering changes of density matrices of electrons constructed from the vectors before and after the connection of molecules.

The fields of mathematics which are important for these studies are mainly functional analysis, theory of numerical analysis based on functional analysis, and the theory of matrix. It seems to be necessary for the study to read and understand the literature in these fields. Moreover, theories and experimental

results that are not formulated in mathematically rigorous ways would also be important as preliminary knowledge for mathematical studies. Therefore, I would like to assimilate the knowledge from the literature. I would like to keep making efforts to solve the long-standing unsolved problems as above finding new principles through trial and error not giving up even in the frontiers.