

My research subject is the many-body problem of the Schrödinger equation, that is, the problem to determine states of N particles based on the Schrödinger equation for large natural number N . Here I consider large yet finite N , and the problem is different from that of the limit as N tends to infinity. Such a problem has been studied from the beginning of quantum mechanics. The characteristic of my research is to try to derive results only on the basis of the Schrödinger equation which is a partial differential equation by mathematically rigorous arguments and to study methods to estimate solutions as quantitative values rather than qualitative behaviors of the solutions and estimate errors of the methods quantitatively. I mainly use the technique called functional analysis which defines sets of functions based on the Lebesgue integral, regard differential operators as mappings between function spaces, and estimate solutions based on properties of the mappings. The differential operator that appears in the Schrödinger equation is specially called Hamiltonian. The spectral theory that has developed through the analysis of the Hamiltonian is a strong investigative tool for the study of the Schrödinger equation. The spectral theory is a natural generalization of the theory of eigenvalue problems for matrices. When we generalize matrices to operators on function spaces, the eigenvalues of the matrices are generalized to spectrum. Spectra include eigenvalues, but there exist spectra called continuous spectra that are not eigenvalues. Elements in function spaces are classified based on the spectrum: eigenfunctions correspond to eigenvalues and scattering states correspond to the continuous spectra.

The operator called scattering matrix which maps the past state to the future state plays an important role in the study of scattering states. I obtained a new definition of the scattering matrix in many-body problems. This is based on a method in which the future state and the past state are considered regarding a time-independent stationary solution as a scattered wave. In one-body problems this method is well known, and the differential cross section which is the radial distribution of the scattering direction is obtained by this method. However, in many body problems the stationary definition is difficult, and there had been only the time-dependent definition. Moreover, I also proved that the new stationary definition is equivalent to the time-dependent definition and gives the same scattering matrix. This result describes the experiments of scattering caused by collisions of molecular beams and is useful for the study of molecular reactions.

The particles treated by the Schrödinger equation are usually electrons and nuclei. Because the mass of an electron is much smaller than that of a nucleus, when we choose an appropriate system of units, the ratio of the masses appears as a small parameter in the Schrödinger equation. The method to study the asymptotic behaviors of solutions as the ratio of masses tends to 0 is called the Born-Oppenheimer approximation. I have also analyzed the Schrödinger equation on the basis of the Born-Oppenheimer approximation. The advantage of the Born-Oppenheimer approximation is its ability to deal with electronic and nuclear motions separately. As for the nuclear motion, I analyzed the motion of an atom in constant magnetic fields and dissociation of molecules mathematically. In these studies, the methods called semiclassical approximation and WKB approximation justified in mathematically rigorous ways that consider asymptotic behaviors of solutions as the parameter in the equations tends to 0 are used. In particular, the result which gives the precise lifetime of a molecule that will dissociate is important for studies of chemical reactions etc.

On the other hand, as for the electronic state I studied the Hartree-Fock equation which is used to obtain electronic states and eigenvalues, and also studied the electronic density. The Hartree-Fock equation is the equation which is satisfied by the critical points of the Hartree-Fock functional, and it is important for the research of the Hartree-Fock equation to study the distribution of the critical values and the critical points of the Hartree-Fock functional. I studied the distribution of the critical values of the Hartree-Fock functional and proved that there exist only a finite number of critical values below a certain threshold. I also proved that the set of all critical points associated with a critical value smaller than the threshold is composed of a finite number of sets called compact connected real-analytic spaces. In these studies, I established a method to show the Fredholm property of the second derivatives of the functionals, and using this method I proved that the sequence of functions obtained by the self-consistent field (SCF) method which is a standard numerical analysis method for the Hartree-Fock equation converges. This is the first important result that ensures the validity of the SCF method theoretically.

Electronic density is the function obtained by integrating the squared absolute value of the eigenfunction of electrons with respect to all variables except for one, and it indicates the expectation value of the number of electrons found in a neighborhood of the point of the variable. I proved very generally that the concentration of electrons in a region is prohibited because of the repulsive interaction between the electrons by showing that the electronic density obtained from the eigenfunction of the Schrödinger equation for electrons in a molecule satisfies an a priori upper bound in a bounded region.