Quantum field theory is known to be the most fundamental theory in the present knowledge. This theory is believed to be the most correct one currently. As a result, this theory is very precise; for example, the prediction of the anomalous magnetic dipole moment of electron shows extreme accordance with experimental observations.

Quantum field theory is extremely successful in perturbative calculations for free particles, while it has not been satisfactory for bound states. The application to bound states is intensely studied, and the sophisticated calculation method has not been established due to its nonperturbativity. The exact simulation of field theory is performed by lattice calculation, such as lattice QCD. However, QED is not included for the lattice computation, since the way to take the continuum limit has not been established. In this work, we consider molecules and atoms as our target. For these bound states, QED plays an important role to bind them.

For the description of the bound states in QED, some treatments, Bethe-Salpeter formalism or NRQED, are frequently discussed. As another approach, in quantum chemistry, the QED correction to Hamiltonian for ab initio calculation is often used, and however the photon is treated as potential in most studies. We want to be able to treat the photon as a particle, for example for the purpose of the study of the quantum system with single photon.

In this work, we propose a new computation method of the time evolution of quantum systems based on QED and report the progress of the development of our program code, QEDynamics [1]. In our method, the operators of quantum fields are treated in Heisenberg picture. The operators are expanded by functions, which are the wave functions computed by the method of quantum chemistry. The expansion is not restricted to the linear terms, since the order of the operator expansion increases by interactions. The evolution of the operators are calculated as the coefficients of the expansion polynomials. Since the aim of our work is the study of bound states, such as molecules, nuclei as well as electrons are treated as quantum fields. In the true theory of physics, parton contributions should be taken into account, such as quarks and gluons, and however we use nuclei for simplicity. The QED including nuclei is formulated with the gauge invariance as Rigged QED [2].
