Solving the Schrödinger equations of interstellar molecules

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Schrödinger equation is the most fundamental equation in quantum mechanics and it governs most of phenomena in molecular science including space chemistry of interstellar molecules. In spite of that importance, however, the exact solutions of this equation have not been able to be solved for over 80 years. Recently, Nakatsuji was successful to propose a new general theory, the free complement (FC) method, for solving this equation [1] and theory was also extended to solving the relativistic Dirac equation [2]. In the tests with a few electron systems, the extremely accurate results could be obtained [3] and the stringent tests of the exactness of the obtained wave functions indicate how accurately the FC wave function can provide close to the exact solutions [4]. With different from ordinary quantum chemistry, the FC method is based on the idea that the exact wave function should be obtained by a functional of the Hamiltonian. Therefore, the adequate wave functions are automatically generated by the system's Hamiltonian itself and this feature is significant for space chemistry that appears the various unusual situations and environments.

We have applied the present method to various atoms and molecules [5] and also interstellar species with the environments of space. In the latter case, the following situations are rather significant: the accurate excited states and theoretical spectra, non Born-Oppenheimer (non-BO) calculations which include the quantum effect of nuclear motion [6], solving the relativistic Dirac equation [2], and atoms and molecules in an extreme environment such as under the strong magnetic fields [7]. For example, the non-BO calculations can provide the vibronic and rotational states including all the quantum effects of electron and nuclear motion, whose theoretical results are directly comparable with the observations and/or experimental results. For the last topic, the Universe's strongest magnetic field was observed on Magnetar object surface in space and the quantum mechanical calculations in magnetic fields become realistically important.

Thus, the present method indicated a high potentiality to be helpful for doing space chemistry in Schrödinger accuracy. We now continue to develop the methods and computational algorithms to be more easily applicable to more general atoms and molecules.

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