Solving the Schrödinger equations of small atoms and molecules with the free complement theory

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The free complement (FC) theory proposed by Nakatsuji in 2004 opens a significant new direction in quantum chemistry, that would make it possible to solve physical and chemistry phenomena with the exact solutions of the Schrödinger equation. We have applied the FC theory to various atoms and molecules and numerically proved its powerful reliability with their highly accurate solutions of the Schrödinger equations. In this talk, the following specific topics will be presented.

1. Non-Born-Oppenheimer (Non-BO) calculations and vibronic and rotational spectra of hydrogen molecular ion and its analytical potential energy curves.
2. Non-BO FC theory applied to some small molecules with their isotopomers by the sampling-based local Schrödinger equation (LSE) method.
3. Accurate calculations of the relativistic Dirac-Coulomb equation of helium atom by proposing the complex-rotated inverse Hamiltonian method without encountering unphysical instabilities.
4. Applications to atoms and molecules in the Universe-level extremely strong magnetic fields.
5. Variational FC s_{ij}-assisted r_{ij} calculations over the Slater functions applied to the $^5S^o$ state of a carbon atom.
6. Recent applications of the FC-LSE theory to some small interstellar species like CH^+, H_4, etc. with their essentially exact potential energy surfaces.