Quantum Chemistry in Schrödinger Accuracy

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Quantum principles represented by the Schrödinger equation and Dirac-Coulomb equation have vast and strong quantitative predictive powers. However, this was not realized for over 80 years, because we did not have a general method of solving these equations in high accuracy. However, recently, this author has found such method [1-3] and one major subject of our QCRI has been to develop efficient methodology. To make theoretical quantum science to be truly predictive, we have to establish accurate and useful method of solving these equations for our common molecular systems.

The accuracy and reliability of our methodology were well established for rather small atoms and molecules. For few-electron systems, like helium, we could give numerical proof on how accurate is our methodology, not only for ground state [4] but also for excited states [5], and not only for energy, but also for wave function itself, like local energy, cusp, and other properties [6]. This was so not only for non-relativistic Schrödinger case, but also for relativistic Dirac-Coulomb case [7]. It was further extended to non-BO case [8]. Though this was done mostly using variation principle where we have to calculate analytical integrals, we have also proposed LSE (local Schrödinger equation) method [9] which is integration-free method and completely general for any analytical functions that are generated automatically by the Hamiltonian of the system (free complement methodology). Further, we have introduced useful local sampling method, anti-symmerization method, and from-atom-to- molecule idea. These methods certainly contributed to increase the atomic and molecular size to which our theory is applicable.

Here, we will introduce some new ideas and formulations on this line of research and show some computational results.

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