

Professor Hiroshi NAKATSUJI

Structure of the Exact Wave Function and a Method of Solving the Schrödinger Equation

*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan
and Fukui Institute for Fundamental Chemistry, Kyoto University, 34-4 Takano-Nishihiraki-cho, Sakyou-ku, Kyoto 606-8103, Japan*

To develop a general systematic method of solving the Schrödinger equation and the corresponding relativistic equation is of a central importance in theoretical physics and chemistry because of its extreme scientific and practical importance. We have investigated the structure of the exact wave function and proposed the methods of calculating the exact wave function [1-6]. Here, after briefly introducing these studies, I will propose the scaled Schrödinger equation that is equivalent to the original Schrödinger equation [7]. It has the variational principle and the square theorem as the original one does. Using the ICI (iterative CI) and ECC (extended (or extreme) coupled cluster) formalisms, we propose general systematic methods for calculating the exact wave functions of atoms and molecules. The nuclear and electron singularity problems no longer occur in these methods. Test applications to hydrogen atom, helium atom, hydrogen molecule and others are satisfactory, implying high potentiality of the proposed method [7].

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