John C Morrison, J Astrophys Aerospace Technol 2016, 4:3(Suppl)
http://dx.doi.org/10.4172/2329-6542.C1.005

Accurate first-principle calculations of the spectra of diatomic molecules in planetary atmospheres

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A summary will be given of various approaches that can be used for doing numerical Hartree-Fock and many-body calculations on atoms and molecules. The theoretical approaches considered include the multi-configuration Hartree-Fock method and many-body perturbation theory. For light atoms and molecules, more than 98 percent of the correlation energy is due to pair excitations. Because molecules lack spherical symmetry, Schrodinger-like equations for molecules typically involve many more independent variables. While, the Hartree-Fock equations for atoms involve a single radial variable and the two-electron pair equation for atoms involve two radial variables, the Hartree-Fock equations for diatomic molecules involves two independent variables and the pair equation for diatomic molecules involve independent variables. To deal with these problems of higher-dimensionality, my mathematical collaborators and I have developed numerical methods for dividing the variable space into smaller sub-regions in which the equations can be solved independently. This domain de-composition theory is described and numerical results are given for Hartree-Fock calculations for diatomic molecules and for numerical solutions of the first-order pair equations which can be used to evaluate the Goldstone diagrams that arise in many-body calculations of molecular spectra. The goal of our calculations is to describe the energy of two helium atoms approaching each other in a cold atomic collision and to obtain the spectral fingerprints of CO and OH molecules in planetary atmospheres.

Biography

John C Morrison has received his PhD in Physics from Johns Hopkins University. After working as a Research Associate at the Argonne Laboratory, he moved to Sweden where he received a number of grants from the Swedish Research Council to build a research group in Theoretical Atomic Physics at Chalmers University of Technology, Sweden. His research in Sweden led to the publication of the monograph "*Atomic Many-body Theory*", which originally appear as volume 13 of the Springer series. The second edition of the book, which was published as volume 3 of the Springer Series on Atoms and Plasmas, has become a Springer classic. He has worked as a Faculty Member in the Department of Physics and Astronomy at the University of Louisville, where he continues to carry on research in Atomic and Molecular Physics. The second edition of his recent textbook, "*Modern Physics for Scientists and Engineers*" (Elsevier, 2015), is based on his teaching of Modern Physics and Quantum.

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