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Numerical Hartree-Fock and correlation calculations of the properties of diatomic molecules

A summary will be given of various approaches that can be used for doing first-principle calculations on atoms and molecules. The theoretical approaches considered include the multi-configuration Hartee-Fock method and many-body perturbation theory. Because molecules lack spherical symmetry, the orbital 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 five independent variables. To deal with these problems of higher-dimensionality, our mathematical collaborators have developed numerical methods for dividing the variable space into smaller sub-regions in which the equations can be solved independently. This domain decomposition theory is described and numerical results are given for Hartree-Fock calculations for diatomic molecules and for numerical solutions of the first-order pair equation, 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 levels and transition probabilities of diatomic molecules to a high level of accuracy. In our contributed paper in this conference, we will show how such methods can be used to calculate the energy of two helium atoms approaching each other in cold atomic collisions 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 in Gothenburg, 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 on Chemical Physics. 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. Returning to USA in 1983, he obtained a Faculty Position in the Department of Physics and Astronomy in 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 mechanics at University of Louisville. His research interests include Theoretical Atomic and Molecular Physics with applications particularly in Astrophysics.

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