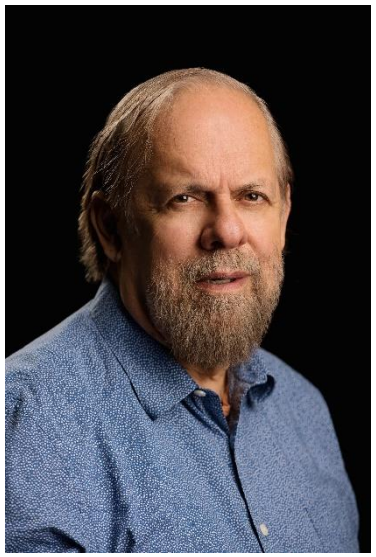
UNIVERSIDAD DE COSTA RICA

CIMPA Centro de Investigación en Matemática Pura y Aplicada

Seminario de Investigación

"Numerical Hartree-Fock and Many-Body Calculations for Diatomic Molecules"



John Morrison, PhD
University of Louisville

John Morrison obtained a position in the Department of Physics and Astronomy at University of Louisville where he has taught courses in elementary physics, astronomy, modern physics, quantum mechanics, and computational physics. His teaching of modern physics in Louisville led to the publication of the book, Modern Physics for Scientists and Engineers (Elsevier, 2010, 2nd Edition 2015). In recent years, he has traveled extensively in The United States, Europe, Latin America, and the Middle East maintaining contacts with scientists and mathematicians at the Colorado School of Mines, the Autonomous University of Mexico, Nicholas Copernicus University in Poland, the University of Buenas Aires in Argentina, and the Hebrew University in Jerusalem.

He is currently teaching a course on modern physics that has a strong computational component in the Physic School of the University of Costa Rica.

Miércoles 14 de noviembre, 2018 – 4:00 p.m.
Mini auditorio, Edificio CIMPA-EMA

Resumen:

The Hartree-Fock theory for diatomic molecules and a theoretical approach for performing many-body calculations are described. Using single-electron wave functions and energies produced by a numerical Hartree-Fock program, the Goldstone diagrams that arise in a perturbation expansion of the energy are evaluated by expressing the Goldstone diagrams in terms of pair functions that are the solution of first-order pair equations. The relevant pair equations are discretized and solved using the spline collocation method with a basis of third-order Hermite splines. Both the Hartree-Fock theory and many-body theory are more complex for diatomic molecules than they are for atoms. 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 involves five independent variables. To deal with these problems of higher-dimensionality, we have developed numerical methods for dividing the variable space into smaller subregions in which the equations can be solved independently. This domain decomposition theory is described and numerical results are given for a single-electron model problem and for many-body calculations for diatomic molecules. Because the long-range goal of our work is to develop an extensive program for doing numerical coupled- cluster calculations on molecules, we will take special care to show how each part of our numerical approach is tested.