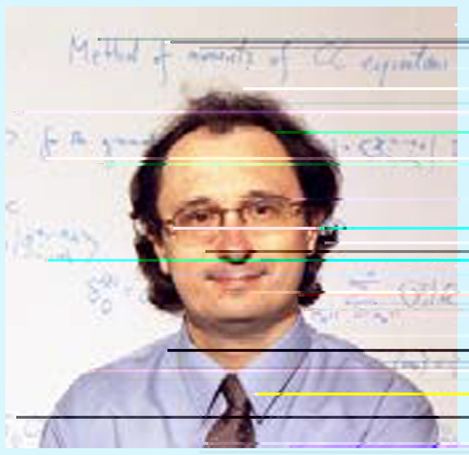
INTRODUCTION TO THE SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY AND ITS DIAGRAMMATIC REPRESENTATION



Speaker: Prof. Piotr Piecuch

Invited by: Prof. Jian Liu

Michigan State University, Michigan 48824, USA

Abstract

The key to a successful description of atoms, molecules, and condensed matter systems is an accurate determination of many-electron correlation effects. Independent-particle-model approximations, such as the Hartree-Fock method that approximates the many-electron wave function by a single Slater determinant, are usually inadequate. In this short course, we will focus on the single-reference MBPT formalism and its diagrammatic representation, which will allow us to understand the mathematical and physical content of many-electron wave functions, while introducing some of the most fundamental and beautiful theorems of quantum many-body theory, including linked and connected cluster theorems.

Content

1. Preliminaries: molecular electronic Schrödinger equation, Slater determinants, CI wave function expansions, and elements of second quantization.
2. Rayleigh-Schrödinger perturbation theory, wave operators, and reference and solvent operators.
3. Eigenfunction and eigenvalue expansions, renormalization terms, and bracketing technique.
4. Diagrammatic representation, rules for MBPT diagrams.
5. MBPT diagrams in low orders (second-, third-, and fourth-order energy corrections; first- and second-order wave function contributions).
6. Linked, unlinked, connected, and disconnected diagrams; diagram cancellations in fourth-order energy and third-order wave function corrections.
7. Linked and connected cluster theorems and their implications.
8. (time permitting, optional) Basic elements of the coupled-cluster theory.

Mini-course 11月12-14日, 15:30-17:30, [illegible]