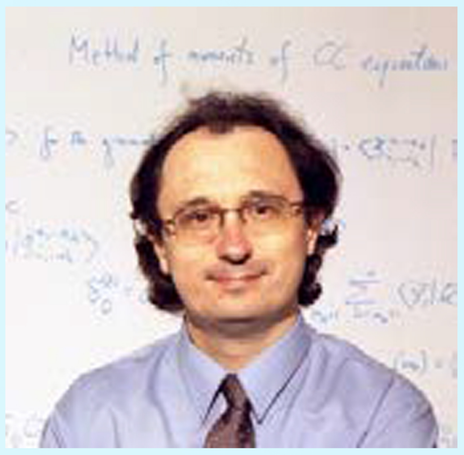
INTRODUCTION TO THE SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY AND ITS DIAGRAMMATIC REPRESENTATION



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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 the 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, reaction, and reduced resolvent 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，北大化学院B229