ALGEBRAIC AND DIAGRAMMATIC METHODS FOR MANY-FERMION SYSTEMS

SPRING 2023, CEM 993: Advanced Topics in Quantum Chemistry

Instructor:
Professor Piotr Piecuch, Department of Chemistry, Michigan State University.
Email: piecuch at chemistry dot msu dot edu.
Websites: https://www.chemistry.msu.edu/faculty-research/faculty-members/piecuch-piotr.aspx (department) and https://www2.chemistry.msu.edu/faculty/piecuch/ (group).
Course website:
http://www2.chemistry.msu.edu/courses/cem993/SS23/syllabus-CEM993-SS23.htm

Course Outline

1. The Second Quantization Formalism
- 1.1. Many-fermion wave functions and spaces, occupation number representation
- 1.2. Creation and annihilation operators, number operator
- 1.3. Anti-commutation relations
- 1.4. Operators in the second-quantized form
- 1.5. Spin-independent operators
- 1.6. Fock space

2. Wick's Theorem
- 2.1. Normal product and contraction of operators
- 2.2. Basic rules for *n*-products and contractions
- 2.3. Derivation of Wick's theorem
- 2.4. Generalized Wick's theorem
- 2.5. Examples: Vacuum mean values of operator products, matrix elements of one- and two-body operators, etc.

3. Hole-Particle Formalism
- 3.1. Fermi vacuum, hole-particle operators
- 3.2. Anti-commutation relations
- 3.3. Normal product and contraction of operators
- 3.4. Wick's theorem in terms of *N*-products
- 3.5. Normal product form of operators
- 3.6. Examples: matrix elements of one- and two-body operators, etc.

4. Diagrammatic Methods
- 4.1. Basic concepts
- 4.2. Skeletons and weights, equivalent diagrams
- 4.3. Graphical representation of operators, Goldstone, Hugenholtz, and Brandow diagrams
- 4.4. Wick's theorem in diagrammatic form, rules for resulting diagrams
- 4.5. Rules for resulting diagrams for spin-independent operators
- 4.6. Summary of rules and examples

5. Independent-Particle-Model Approximation
- 5.1. Thouless theorem
- 5.2. Hartree-Fock equations
- 5.3. Brueckner orbitals

6. Many-Body Perturbation Theory (MBPT)
- 6.1. Rayleigh-Schrödinger perturbation theory, wave, reaction, and reduced resolvent operators
- 6.2. Eigenfunction and eigenvalue expansions, renormalization terms, and bracketing technique
- 6.3. Diagrammatic representation, rules for MBPT diagrams
- 6.4. MBPT diagrams in low orders (second, third, and fourth-order energy contributions; first and second-order wave function contributions)
- 6.5. Linked, unlinked, connected, and disconnected diagrams
- 6.6. Exclusion Principle Violating (EPV) diagrams
- 6.7. Factorization Lemma
- 6.8. Linked Cluster Theorem
- 6.9. Connected-Cluster Theorem
- 6.10. Summary of the rules for constructing MBPT diagrams in any order

7. Coupled-Cluster Theory
- 7.1. Coupled-cluster exponential wave function ansatz
- 7.2. Diagrammatic representation
- 7.3. Connected and disconnected clusters
- 7.4. Connected-cluster form of the Schrödinger equation and general coupled-cluster equations
- 7.5. Approximate coupled-cluster methods: the CCD, CCSD, CCSDT, and CCSDTQ approaches
- 7.6. Diagrammatic derivation of the CCD and CCSD equations
- 7.7. Relationship with configuration interaction (CI) and MBPT theories.
- 7.8. New developments in coupled-cluster theory and future outlook.