CHEM 580/PHYSICS 580: Special Topics in Physical Chemistry (Spring 2016)

ALGEBRAIC AND DIAGRAMMATIC METHODS FOR MANY-FERMION SYSTEMS

Classes: MWF 8:30 a.m.-10:00 a.m. (with 10-minute break), Room 301, Laboratory Sciences Bldg. The first lecture on January 20, 2016 will start at 9:00 a.m. All of the remaining lectures will start at 8:30 a.m.
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Course website: https://pages.wustl.edu/ppiecuch.

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.