Lecture 1:

Introductory remarks; many-particle Schrödinger equation; molecular, electronic, and nuclear Hamiltonians; antisymmetric wave functions for many-fermion systems; single-particle states/spin-orbitals.

Lecture 2:

Slater determinants; expansions of many-fermion wave functions in terms of Slater determinants (full configuration interaction expansions); occupation number representation; creation and annihilation operators; true vacuum state; number operator.

Lecture 3:

Anti-commutation relations for creation and annihilation operators and their consequences; many-particle operators in second-quantized form (part I).

Lecture 4:

Many-particle operators in second-quantized form (part II); non-symmetric vs. antisymmetrized matrix elements.

Lecture 5:

Many-particle operators in second-quantized form (part III); spin-independent operators in electronic structure theory; normal product of operators; contraction of operators; normal product with contractions.

Lecture 6:

Basic rules for normal products without and with contractions, when acting on the vacuum state and when forming expectation values in the vacuum state; derivation of Wick's theorem (part I).

Lecture 7:

Derivation of Wick's theorem (part II).

Lecture 8:

Generalized Wick's theorem; basic rules for operator products, when acting on the vacuum state and when forming expectation values in the vacuum state; matrix elements involving Slater determinants.

Lecture 9:

Applications of Wick's theorem: matrix elements of one- and two-body operators involving Slater determinants (part I).

Lecture 10:

Applications of Wick's theorem: matrix elements of one- and two-body operators involving Slater determinants (part II); introductory remarks about hole-particle formalism; reference and excited determinants; Fermi vacuum state; occupied or hole and unoccupied or particle states; particle-hole excitation operators and their usefulness in representing many-fermion wave functions; hole-particle creation and annihilation operators.

Lecture 11:

Anti-commutation relations for hole-particle creation and annihilation operators; normal products, contractions, and normal products with contractions with respect to Fermi vacuum.

Lecture 12:

Wick's theorem and generalized Wick's theorem in hole-particle formalism; basic rules for operator products, when acting on the Fermi vacuum state and when forming expectation values in the Fermi vacuum state; matrix elements of one- and two-body operators involving Slater determinants revisited (part I).

Lecture 13:

Matrix elements of one- and two-body operators involving Slater determinants revisited (part II); many-particle operators in normal product form (part I).

Lecture 14:

Many-particle operators in normal product form (part II); normal-ordered form of the Hamiltonian; usefulness of normal ordering in evaluating matrix elements of many-body operators; basic concepts of diagrammatic approach (part I).

Lecture 15:

Basic concepts of diagrammatic approach (part II): diagrammatic representation of creation and annihilation operators and their contractions using external and internal Fermion lines, simple and super-vertices representing many-body operators in Goldstone representation, left-right orientation convention for hole and particle Fermion lines, free (i.e., summation) vs. fixed indices in a diagram, graphical representation of many-body operator expressions in terms of sign, weight, and scalar factors, and operator parts, products of many-body operators as diagrams along the time axis.

Lecture 16:

Basic concepts of diagrammatic approach (part III): free (i.e., summation) vs. fixed indices in labeling internal Fermion lines, resulting vs. admissible resulting diagrams, rules for resulting diagrams representing expectation values of operator products in the Fermi vacuum state and products of operators acting on the Fermi vacuum state, summary of key steps of diagrammatic calculations, initial examples illustrating basic diagrammatic concepts.

Lecture 17:

More examples illustrating basic diagrammatic concepts; equivalent vs. non-equivalent resulting diagrams.

Lecture 18:

Final examples illustrating basic diagrammatic concepts (prior to discussion of skeletons and weights in Goldstone and Hugenholtz representations planned for lecture 19).

Lecture 19:

Oriented skeletons; Goldstone vs. Hugenholtz representations; significance of equivalent loops and equivalent open paths in weight determination in Goldstone representation; significance of equivalent Fermion lines in weight determination in Hugenholtz representation; group of automorphisms, equivalence classes, and topological factor of a skeleton; weight of a diagram (or a skeleton) as an inverse of a topological factor; connected and disconnected diagrams.

Lecture 20:

Weight determination for disconnected diagrams; summary of rules for determining weights of diagrams (or oriented skeletons); proof of theorem that relates the number of distinct ways of forming a resulting diagram with the weights of the resulting and component diagrams..

Lecture 21:

Proof of diagrammatic analog of generalized Wick's theorem (part I); significance of loops and internal hole lines in sign determination.

Lecture 22:

Proof of diagrammatic analog of generalized Wick's theorem (part II); additional rules for diagrams representing products of operators in standard (as opposed to normal-ordered) form; interpretation of resulting diagrams representing expectation values of operator products in the Fermi vacuum state and products of operators acting on the Fermi vacuum state; examples illustrating the use of diagrammatic rules.

Lecture 23:

Hugenholtz vs. Goldstone diagrams; determination of sign factors in diagrammatic work using Hugenholtz representation via Brandow diagrams; summary of key steps of diagrammatic calculations employing Hugenholtz representation; Hugenholtz skeletons and diagrams as intermediate steps in determining Goldstone resulting diagrams; more examples illustrating the use of diagrammatic rules.

Lecture 24:

Usefulness of Goldstone representation in calculations involving spin-independent operators; independent-particle-model approximations; Thouless theorem.

Lecture 25:

Proof of Thouless theorem.

Lecture 26:

Hartree-Fock theory; derivation of Hartree-Fock equations using a combination of variational approach, Thouless theorem, and diagrammatic methods; examination of Hartree-Fock equations and their solutions; self-consistent-field procedure; symmetry-adapted vs. symmetry-broken solutions; Löwdin's symmetry dilemma.

Lecture 27:

More remarks about symmetry-adapted vs. symmetry-broken solutions of Hartree-Fock equations; Brueckner maximum overlap orbitals; introductory comments about many-body perturbation theory (MBPT) as a method to solve the many-fermion Schrödinger equation.

Lecture 28:

Introductory remarks about many-body perturbation theory (MBPT) as a method to solve the many-fermion correlation problem; Rayleigh-Schrödinger perturbation theory for a Hermitian, nondegenerate, eigenvalue problem (part I): unperturbed and perturbed eigenvalue problems, intermediate normalization, wave, reaction, and reduced resolvent operators, bracketing function, expressions for perturbed eigenstate and eigenvalue in terms of reduced resolvent operator.

Lecture 29:

Rayleigh-Schrödinger perturbation theory for a Hermitian, nondegenerate, eigenvalue problem (part II): more information about bracketing function and expressions for perturbed eigenstate and eigenvalue in terms of reduced resolvent operator, Bloch wave operator and its properties (a nondegenerate case), final working expressions for wave and reaction operators used in perturbation theory, power series expansions defining wave and reaction operators and the analogous power series expansions defining target eigenstate and eigenvalue in terms of unperturbed reduced resolvent and perturbation operators.

Lecture 30:

Rayleigh-Schrödinger perturbation theory for a Hermitian, nondegenerate, eigenvalue problem (part III): more information about power series expansions defining wave and reaction operators and the analogous power series expansions defining target eigenstate and eigenvalue in terms of unperturbed reduced resolvent and perturbation operators, spectral (sum-over-states) representation of unperturbed reduced resolvent, examples of expressions for perturbative corrections to the wave function/wave operator and energy/reaction operator (the lowest four orders).

Lecture 31:

Rayleigh-Schrödinger perturbation theory for a Hermitian, nondegenerate, eigenvalue problem (part IV): expressions for perturbative corrections to the wave function and energy using spectral representation of unperturbed reduced resolvent, principal and renormalization terms, bracketing technique of Brueckner and Huby; return to many-body perturbation theory (MBPT).

Lecture 32:

Details of many-body perturbation theory (MBPT; part I): decomposition of normal-ordered Hamiltonian into unperturbed Hamiltonian and perturbation, Slater determinants as unperturbed eigenstates, single-particle energies and single-particle excitation energies as building blocks for unperturbed energies, many-body structure of perturbation operator, unperturbed reduced resolvent in MBPT and its many-body components.

Lecture 33:

Details of many-body perturbation theory (MBPT; part II): diagrammatic representation of many-body components of perturbation operator and unperturbed reduced resolvent, examination of the second-order MBPT (MBPT(2)) correction to the energy, initial observations regarding the elimination of reduced resolvent diagrams via the rule defining MBPT denominators.

Lecture 34:

Details of many-body perturbation theory (MBPT; part III): diagrams and explicit expressions representing the second-order MBPT (MBPT(2)) correction to the energy and the first-order MBPT (MBPT(1)) correction to the wave function and their physical interpretation, elimination of reduced resolvent diagrams via the rule defining MBPT denominators, rules for constructing and interpreting energy and wave function diagrams in MBPT.

Lecture 35:

Details of many-body perturbation theory (MBPT; part IV): summary of rules for MBPT energy and wave function diagrams, the third-order MBPT (MBPT(3)) correction to the energy and its physical content, time versions of MBPT diagrams.

Lecture 36:

Details of many-body perturbation theory (MBPT; part V): the fourth-order MBPT (MBPT(4)) correction to the energy and its physical content, cancellation of disconnected diagrams originating from the principal term and diagrams representing the renormalization terms in the MBPT(4) energy correction, statement of linked-cluster theorem for MBPT energy corrections in any order, the second- and third-order MBPT corrections to the wave function and their physical content, initial remarks about linked and unlinked diagrams.

Lecture 37:

Details of many-body perturbation theory (MBPT; part VI): more information about linked and unlinked diagrams, cancellation of unlinked diagrams originating from the principal term and diagrams representing the renormalization terms in the third- and fourth-order wave function corrections, statement of linked-cluster theorem for MBPT wave function corrections in any order, exclusion principle violating (EPV) diagrams and their significance for linked-cluster theorem.

Lecture 38:

Details of many-body perturbation theory (MBPT; part VII): more information about exclusion principle violating (EPV) diagrams and their significance for linked-cluster theorem, factorization of disconnected linked diagrams, preliminary discussion of factorization theorem.

Lecture 39:

Details of many-body perturbation theory (MBPT; part VIII): proof of factorization theorem by Frantz and Mills, proof of linked-cluster theorem of Brueckner and Goldstone (initial steps).

Lecture 40:

Details of many-body perturbation theory (MBPT; part IX): proof of linked-cluster theorem of Brueckner and Goldstone (continuation and final steps), significance of linked-cluster theorem for size-extensivity of MBPT energy corrections.

Lecture 41:

Linked character of many-fermion wave functions resulting from finite- and infinite-order MBPT considerations; cluster operator and its MBPT structure; significance of many-body components of the cluster operator; proof of connected-cluster theorem of Hubbard and Hugenholtz; exponential wave function ansatz of coupled-cluster theory.

Lecture 42, Part I:

Review of Lecture 41, especially, the connected-cluster theorem of Hubbard and Hugenholtz; introductory remarks about coupled-cluster theory, including various arguments in favor of the exponential wave function ansatz; CCSD, CCSDT, CCSDTQ, etc. hierarchy; comparison of configuration interaction and coupled-cluster expansions for the wave function; cluster analysis of many-fermion wave functions; lowest MBPT orders in which various connected and disconnected clusters contribute to the wave function and energy; comparisons of truncated coupled-cluster, configuration interaction, and MBPT approaches (CCSD, CCSDT, CCSDTQ vs. CISD, CISDT, CISDTQ vs. MBPT(2), MBPT(3), MBPT(4)) focusing on computational costs vs. accuracy; approximate CCSDT calculations using noniterative triples corrections to CCSD energy (CCSD+T(CCSD), CCSD(T), CR-CC(2,3), and similar approaches).

Lecture 42, Part II:

Initial remarks about coupled-cluster equations; problems with nonterminating series that represents the expectation value of the Hamiltonian using the exponential wave function ansatz; the single-reference coupled-cluster theory of Coester, Kümmel, Čížek, and Paldus as a practical alternative to (generally impractical) variational considerations; selected technical details of the single-reference coupled-cluster theory: connected-cluster form of the Schrödinger equation and its diagrammatic derivation (Čížek), derivation of the connected-cluster form of the Schrödinger equation using commutator expansion of the similarity-transformed Hamiltonian (Coester), coupled-cluster energy and amplitude equations as projections of the connected-cluster form of the Schrödinger equation on the reference and excited determinants, derivation of the explicit formula for the coupled-cluster energy in terms of matrix elements of the Hamiltonian in the normal-ordered form and singly and doubly excited cluster amplitudes, general recipe for deriving coupled-cluster amplitude equations, beginning of the diagrammatic derivation of CCD amplitude equations (nonoriented skeletons, Hugenholtz diagrams, Brandow diagrams up to linear terms).

Lecture 42, Part III:

Conclusion of the diagrammatic derivation of CCD amplitude equations (the remaining Brandow diagrams for nonlinear terms, algebraic expressions in terms of matrix elements of the Hamiltonian in the normal-ordered form and doubly excited cluster amplitudes); final remarks: solving coupled-cluster equations using CCD amplitude equations as an example; understanding CPU operation count for various terms in coupled-cluster amplitude equations; achieving efficiency of coupled-cluster computer codes via diagram factorization and recursively generated intermediates using CCD and CCSD equations as examples.