Mathematical methods in quantum chemistry I.

I. Basic ideas

1. Variational principle
2. Variational theorem
3. Eckart inequivality
4. Mc Donalds theorem
5. Huzinaga type equations
6. The method of moments
7. Energy expressions
   a) Rayleigh quotient
   b) Transition formula
   c) Local energy
   d) Horn - Weinstein formula
8. The antisymmetrizer
9. Expansion theorem

II. Perturbation theory (PT)

1. n-th order Rayleigh - Schrödinger results: recursive formulae
2. Helmann - Feynman theorem
   a) differential
   b) integral
3. Unsøld approximation
4. Wigner 2n+1 theorem
5. Adiabatic coupling
6. The reduced resolvent
7. Fast derivation of PT
8. Hylleraas functional
9. Brillouin - Wigner PT
10. Extensivity of Rayleigh - Schrödinger PT
11. PT with non-diagonal zero order

III. Löwdin's Partitioning technique

1. Matrix partitioning
2. Partitioning by projectors
3. Schwinger's wave operator. Formal solution of the Schrödinger equation
4. The energy equation
5. Connection to PT
6. Bruckner's reaction operator. Lippmann - Schwinger equation
7. Bloch equation
8. Energy-independent partitioning

IV. Second quantization

1. Wave functions
2. Operators
3. Matrix elements
4. Reduced density matrices
5. Using spatial orbitals
6. Model Hamiltonians
7. Electron-hole symmetry for alternating hydrocarbons
8. The Fockian as an averaged Hamiltonian
9. Brillouin Theorem
10. The Hartree-Fock equations
11. Many-body perturbation theory
12. Laplace transformed denominators in PT
13. Equations for density matrices: contracted Schrödinger equations
14. Coupled cluster theory