

SYLLABUS FOR CHM 7485, 2021, Fall Term. R. J. Bartlett,  
Tuesday, Thursday, 10:40 to noon, New QTP Conference room,  
Leigh, 240 E.

TEXT: Not mandatory but copies should be available.

Isaiah Shavitt and R. J Bartlett,

“Many-Body Methods in Chemistry and Physics:  
MBPT and Coupled-cluster Theory”  
Cambridge Molecular Science

Handout. Bartlett and Musial in “Reviews of  
Modern Physics”.

- I. Why coupled-cluster theory?  
Extensivity. Power of exponential wavefunction.
- II. Systematic development of CC tools.  
Second-quantization  
Normal Ordered Operators  
Wick’s Theorem-Contractions
- III. Coupled-cluster doubles Eqns.  
Algebraic Derivation  
Diagrammatic derivation  
Connections with Perturbation Theory
- IV. CCSD Eqns.
- V. Density Matrices

- VI. CCSDT Eqns.
  - CCSD(T)
  - CCSDTQ<sub>f</sub>
  - CCSDT(Q)
- VII. Distinguished Cluster Approximations
- VIII. Analytic Gradients and Properties
- IX. Equation-of Motion CC Method for Excited States
  - IP/EA-EOM-CC
  - EE-EOM-CC
- X. STEOM-CC
- XI. Hilbert Space-Multi-reference Approach.