FYS.425 (FYS-4706) QUANTUM THEORY OF ELECTRONIC STRUCTURES

Credit units: 5 ECTS

Lectures: 40 h
Tue 10 – 12 SG312
Wed 10 – 12 SG312

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--> FYS-4706 . . . (FYS.425, later)

Exercises: 12 x 2 h
Thu 10 – 12 SG312

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Text book: P.W. Atkins and R.S. Friedman:
Molecular Quantum Mechanics, Chapters 1 – 9
(Fifth edition, OXFORD University Press)

Prerequisites: Basics of physics and chemistry, quantum mechanics helps

Examination: 20.12.21, 8.2.22 and 15.3.22

SCHEDULE 2021

	WEEK		Lectures		Exercises	Note!
August – September	35	Tue	1 – 2			
		Wed	3 – 4	Thu		
	36	Tue	5 – 6			
		Wed		Thu	1	
	37	Tue	7 – 8			
		Wed	9 – 10	Thu	2	
	38	Tue	11 – 12			
		Wed	13 – 14	Thu	3	
	39	Tue	15 – 16			
		Wed	17 – 18	Thu	4	
	40	Tue				
		Wed	19 – 20	Thu	5	
October	41	Tue				
		Wed		Thu	6	
	42					**Exam week**
	43	Tue	21 – 22			
		Wed	23 – 24	Thu		
	44	Tue	25 – 26			
		Wed	27 – 28	Thu	7	
November	45	Tue				
		Wed	29 – 30	Thu	8	
	46	Tue				
		Wed	31 – 32	Thu	9	
	47	Tue	33 – 34			
		Wed	35 – 36	Thu	10	
	48	Tue	37 – 38			
		Wed	39 – 40	Thu	11	
December	49	Tue				
		Wed		Thu	12	
	50			Fri		**Exam week**
	51		Exam 20.12.21	Fri		

CONTENTS

OTHER LITERATURE

Modern and extensive, recommended

Richard M. Martin:
Electronic structure: Basic Theory and Practical Methods
(Cambridge University Press, 2012)

Classical quantum chemistry

M. Weissbluth:
Atoms and Molecules
(Academic Press, New York, 1983)

Jean–Louis Calais:
Quantum Chemistry Workbook
(John Wiley & Sons,New York, 1994)

I. Lindgren och S. Svanberg:
Atomfysik
(Universitetsförlaget Uppsala, LiberTryck Stockholm, 1974)

A. Hinchliffe:
Computational Quantum Chemistry
(John Wiley & Sons,Chichester, New York, 1989)

Jorge Kohanoff:
Electronic Structure Calculations for Solids and Molecules
(Cambridge University Press, 2006)

Density functional theory

R.G. Parr and W. Yang:
Density-Functional Theory of Atoms and Molecules
(Oxford University Press, Oxford, New York, 1989)

Wolfram Koch and Max C. Holthausen:
A Chemist's Guide to Density Functional Theory
(Wiley-VCH, 2001)

T.T. Rantala:
Local-Density Electronic Structure Calculations on the Spectra and Reactivity of Metals
Acta Univ. Ouluensis A 184 (1987)

Classical nanocrystals and nanostructures

S.V. Gaponenko:
Optical Properties of Semiconductor Nanocrystals
Cambridge Studies in Modern Optics
(Cambridge University Press, Cambridge, 1998)

Path integral approaches, technical – not directly related to these lectures

Richard P. Feynman and Albert L. Hibbs:
Quantum Mechanics and Path Integrals
Emended Edition by D.F. Styer
(Dover Publications Inc., Mineola, New York, 2005)

Hagen Kleinert:
Path Integrals in Quantum Mechanics, Statistics, Polymer Physics and Financial Markets
(World Scientific, Fifth Edition, 2009)

L.S. Schulman:
Techniques and Applications of Path Integration
(Dover Publications Inc., Mineola, New York, 2005)

Harald J.W. Müller-Kirsten:
Introduction to Quantum Mechanics: Schrödinger Equation and Path Integral
(World Scientific, 2006)

Papers of **electronic structure calculations** with path integrals from T.T. Rantala *et al.*:
http://iki.fi/trantala/paths