

FYS.425 QUANTUM THEORY OF ELECTRONIC STRUCTURES

(FYS-4706)

Credit units: 5 ECTS

Lectures: 40 h
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 --> FYS-4706 . . . (FYS.425, later)

Exercises: 12 x 2 h
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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			QTES, 2021	ii
	WEEK	Lectures	Exercises	Note!		
August	35	Tue 1 – 2				
		Wed 3 – 4	Thu			
September	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				
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	48	Tue 37 – 38				
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December	49	Tue				
		Wed	Thu 12			
	50				Exam week	
	51	Exam 20.12.21	Fri			

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0.2. Heat capacities 4

0.3. Photoelectric and Compton effects 4

0.4. Atomic spectra 5

0.5. Duality of matter 6

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 1.2. Eigenfunctions and eigenvalues 7

 1.3. Representations 9

 1.4. Commutation and non-commutation 9

 1.5. Construction of operators 10

 1.6. Integrals over operators 11

 1.7. Dirac bracket and matrix notation 12

 1.8. Hermitian operators 15

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"Evolution of Quantum Theory" and other issues	C1

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>