

FYS.425 QUANTUM THEORY OF ELECTRONIC STRUCTURES

(FYS-4706)

Credit units:	5 ECTS	
Lectures:	40 h Tue 10 – 12 SG312 Wed 10 – 12 SG312	Tapio Rantala, prof. SG219 FirstName.LastName@tuni.fi http://iki.fi/trantala/opetus/ --> FYS-4706 . . . (FYS.425, later)
Exercises:	12 x 2 h Thu 10 – 12 SG312	Ilkka Ruokosenmäki FirstName.LastName@tuni.fi
Text book:	P.W. Atkins and R.S. Friedman: <i>Molecular Quantum Mechanics</i> , Chapters 1 – 9 (Fifth edition, OXFORD University Press)	
Prerequisites:	Basics of physics and chemistry, quantum mechanics helps	
Examination:	19.12.22, 7.2.23 and 14.3.23	

SCHEDULE 2022

QTES, 2022

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	WEEK	Lectures	Exercises	Note!	
August	35	Tue 1 – 2 Wed 3 – 4	Thu		
	36	Tue 5 – 6 Wed 7 – 8	Thu 1		
September	37	Tue 9 – 10 Wed 11 – 12	Thu 2		
	38	Tue 13 – 14 Wed 15 – 16	Thu 3		
	39	Tue 17 – 18 Wed 19 – 20	Thu 4		
	40	Tue 21 – 22 Wed 23 – 24	Thu 5		
October	41	Tue 25 – 26 Wed 27 – 28	Thu 6		
	42				Exam week
	43	Tue 29 – 30 Wed 31 – 32	Thu 7		
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November	45	Tue 37 – 38 Wed 39 – 40	Thu 9		
	46	Tue 43 – 44 Wed 45 – 46	Thu 10		
	47	Tue 47 – 48 Wed 49 – 50	Thu 11		
	48	Tue 51 – 52 Wed 53 – 54	Thu 12		
December	49				Exam week
	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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 1.3. Representations 9
 1.4. Commutation and non-commutation 9
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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>