

FDITE219 Numerical Analysis of Time-Dependent Quantum Systems

Description:

The course explores the numerical analysis of time-dependent nonrelativistic quantum dynamics, focusing on solving the Schrödinger equation, diagonalization and integration techniques, and the representation of multipartite systems.

Topics:

Fundamentals of the time-dependent Schrödinger equation (TDSE): norm preservation, time-evolution operator

TDSE expansion in a given basis, dynamics as an initial-value problem for coupled differential equations.

Closed quantum systems: formulation via diagonalization of a time-independent Hamiltonian; numerical diagonalization techniques.

General cases including time-dependent excitation: numerical integration of the TDSE in basis representation; commonly used integration schemes, trade-offs between accuracy and runtime, adaptive step sizing.

Multipartite quantum systems: representation of tensor product spaces.

Examples include two-level systems in classical time-dependent fields, spatial dynamics as partial differential equations with corresponding numerical methods, and treatment of the excited, ionizing hydrogen atom.

Outlook: basic concepts of density functional theory.

Literature:

Wolfgang Schweizer: *Numerical Quantum Dynamics*, Springer, 2002. ISBN: 978-0-306-47617-7

Paolo Giannozzi: *Numerical Methods in Quantum Mechanics* by (Lecture Notes at the University of Udine, <https://www.fisica.uniud.it/~giannozz/Corsi/MQ/LectureNotes/mq.pdf>)

William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery: *Numerical Recipes in C: The Art of Scientific Computing*, 2nd Edition. Cambridge University Press, 1992. ISBN 978-0-521-43108-8.