# Equations of motion derived by Time-Dependent Variational Principle

Time-dependent variational principle (TDVP)

$$\delta S = \delta \int \langle \Phi(t) | i\hbar \partial_t - \hat{H} | \Phi(t) \rangle dt = 0$$

**⇒** 

$$\dot{q} = \frac{\partial H}{\partial p}$$
 ,  $\dot{p} = -\frac{\partial H}{\partial q}$  ,  $\hbar \dot{G} = \frac{\partial H}{\partial \Sigma}$  ,  $\hbar \dot{\Sigma} = -\frac{\partial H}{\partial G}$ 

- -G and  $\Sigma$  appear with  $\hbar$ 
  - · · · describe the dynamics of quantum fluctuations

# Geometry Of The Time Dependent Variational Principle In Quantum Mechanics

**Marc J J Vrakking, Franck Lepine** 

# **Geometry Of The Time Dependent Variational Principle In Quantum Mechanics:**

Geometry of the Time-Dependent Variational Principle in Quantum Mechanics P. Kramer, M. Saraceno, 2014-01-15 Geometry of the time-dependent variational principle in quantum mechanics Peter Kramer, Marcos From Quantum to Classical Molecular Dynamics Christian Lubich, 2008 Quantum dynamics of molecules poses a variety of computational challenges that are presently at the forefront of research efforts in numerical analysis in a number of application areas high dimensional partial differential equations multiple scales highly oscillatory solutions and geometric structures such as symplecticity and reversibility that are favourably preserved in discretizations This text addresses such problems in quantum mechanics from the viewpoint of numerical analysis illustrating them to a large extent on intermediate models between the Schrodinger equation of full many body quantum dynamics and the Newtonian equations of classical molecular dynamics The fruitful interplay between quantum dynamics and numerical Advances in Quantum Chemistry, 2015-01-29 Advances in Quantum Chemistry presents surveys of analysis is emphasized current topics in this rapidly developing field one that has emerged at the cross section of the historically established areas of mathematics physics chemistry and biology It features detailed reviews written by leading international researchers In this volume the readers are presented with an exciting combination of themes Presents surveys of current topics in this rapidly developing field that has emerged at the cross section of the historically established areas of mathematics physics chemistry and biology Features detailed reviews written by leading international researchers **Advances in Quantum Chemistry: Lowdin Volume**, 2017-02-12 Advances in Quantum Chemistry Lowdin Volume presents a series of articles exploring aspects of the application of quantum mechanics to atoms molecules and solids Celebrates Per Olov Lowdin who would have been 100 in 2016 Contains papers by many who use his ideas in theoretical chemistry and physics today *Ouantum Chemistry* and Dynamics of Excited States Leticia González, Roland Lindh, 2020-11-10 An introduction to the rapidly evolving methodology of electronic excited states For academic researchers postdocs graduate and undergraduate students Quantum Chemistry and Dynamics of Excited States Methods and Applications reports the most updated and accurate theoretical techniques to treat electronic excited states From methods to deal with stationary calculations through time dependent simulations of molecular systems this book serves as a guide for beginners in the field and knowledge seekers alike Taking into account the most recent theory developments and representative applications it also covers the often overlooked gap between theoretical and computational chemistry An excellent reference for both researchers and students Excited States provides essential knowledge on quantum chemistry an in depth overview of the latest developments and theoretical techniques around the properties and nonadiabatic dynamics of chemical systems Readers will learn Essential theoretical techniques to describe the properties and dynamics of chemical systems Electronic Structure methods for stationary calculations Methods for electronic excited states from both a quantum chemical and time dependent point of view A

Introduction to Modern Methods of Quantum Many-body Theory and Their Applications A. Fabrocini, Stefano Fantoni, Eckhard Krotscheck, 2002 The book contains pedagogical articles on the dominant non stochastic methods of microscopic many body theories Density functional theory coupled cluster theory and correlated basis functions methods in their widest sense Further articles introduce students to applications of these methods in front line research such as Bose Einstein condensates the nuclear many body problem and the dynamics of quantum liquids These keynote articles are supplemented by experimental reviews on intimately connected topics of current relevance The book addresses the striking lack of pedagogical reference literature in the field that allows researchers to acquire the requisite physical insight and technical skills The volume should therefore not only researchers to acquire the requisite physical insight and technical skills The volume should therefore not only serve as a collection of information relevant to those who attended the school but it provides be useful reference material to a broad range of theoretical physicists in condensed matter and nuclear theory

Quantum Mechanics via Lie Algebras Arnold Neumaier, Dennis Westra, 2024-10-07 This monograph introduces mathematicians physicists and engineers to the ideas relating quantum mechanics and symmetries both described in terms of Lie algebras and Lie groups The exposition of quantum mechanics from this point of view reveals that classical mechanics and quantum mechanics are very much alike Written by a mathematician and a physicist this book is like a math book about precise concepts and exact results in classical mechanics and quantum mechanics but motivated and discussed like a physics book in terms of their physical meaning The reader can focus on the simplicity and beauty of theoretical physics without getting lost in a jungle of techniques for estimating or calculating quantities of interest Fundamentals of Nuclear Models David J. Rowe, John L. Wood, 2010 This book reviews the basic models and theories of nuclear structure and gives an in depth analysis of their experimental and mathematical foundations It shows the relationships between the models and exhibits the value of following the strategy of looking for patterns in all the data available developing phenomenological models to explain

them and finally giving the models a foundation in a fundamental microscopic theory of interacting neutrons and protons This unique book takes a newcomer from an introduction to nuclear structure physics to the frontiers of the subject along a painless path It provides both the experimental and mathematical foundations of the essential models in a way that is accessible to a broad range of experimental and theoretical physicists Thus the book provides a unique resource and an exposition of the essential principles mathematical structures assumptions and observational data on which the models and theories are based It avoids discussion of many non essential variations and technical details of the models Schrödinger Dynamics of Bose-Einstein Condensates Kaspar Sakmann, 2011-08-31 At extremely low temperatures clouds of bosonic atoms form what is known as a Bose Einstein condensate Recently it has become clear that many different types of condensates so called fragmented condensates exist In order to tell whether fragmentation occurs or not it is necessary to solve the full many body Schr dinger equation a task that remained elusive for experimentally relevant conditions for many years In this thesis the first numerically exact solutions of the time dependent many body Schr dinger equation for a bosonic Josephson junction are provided and compared to the approximate Gross Pitaevskii and Bose Hubbard theories It is thereby shown that the dynamics of Bose Einstein condensates is far more intricate than one would anticipate based on these approximations A special conceptual innovation in this thesis are optimal lattice models It is shown how all quantum lattice models of condensed matter physics that are based on Wannier functions e g the Bose Fermi Hubbard model can be optimized variationally This leads to exciting new physics Theory and Applications of Computational Chemistry Clifford Dykstra, Gernot Frenking, Kwang Kim, Gustavo Scuseria, 2011-10-13 Computational chemistry is a means of applying theoretical ideas using computers and a set of techniques for investigating chemical problems within which common questions vary from molecular geometry to the physical properties of substances Theory and Applications of Computational Chemistry The First Forty Years is a collection of articles on the emergence of computational chemistry It shows the enormous breadth of theoretical and computational chemistry today and establishes how theory and computation have become increasingly linked as methodologies and technologies have advanced Written by the pioneers in the field the book presents historical perspectives and insights into the subject and addresses new and current methods as well as problems and applications in theoretical and computational chemistry Easy to read and packed with personal insights technical and classical information this book provides the perfect introduction for graduate students beginning research in this area It also provides very readable and useful reviews for theoretical chemists Written by well known leading experts Combines history personal accounts and theory to explain much of the field of theoretical and computational chemistry Is the perfect introduction to the field Density-Functional Methods for Excited States Nicolas Ferré, Michael Filatov, Miquel Huix-Rotllant, 2015-08-26 The series Topics in Current Chemistry presents critical reviews of the present and future trends in modern chemical research The scope of coverage is all areas of chemical science including the interfaces with related

disciplines such as biology medicine and materials science The goal of each thematic volume is to give the non specialist reader whether in academia or industry a comprehensive insight into an area where new research is emerging which is of interest to a larger scientific audience Each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole The most significant developments of the last 5 to 10 years are presented using selected examples to illustrate the principles discussed The coverage is not intended to be an exhaustive summary of the field or include large quantities of data but should rather be conceptual concentrating on the methodological thinking that will allow the non specialist reader to understand the information presented Contributions also offer an outlook on potential future developments in the field Review articles for the individual volumes are invited by the volume editors Readership research chemists at universities or in industry graduate students Coherent Quantum Physics Arnold Neumaier, 2019-10-21 This book introduces mathematicians physicists and philosophers to a new coherent approach to theory and interpretation of quantum physics in which classical and quantum thinking live peacefully side by side and jointly fertilize the intuition The formal mathematical core of quantum physics is cleanly separated from the interpretation issues The book demonstrates that the universe can be rationally and objectively understood from the smallest to the largest levels of modeling The thermal interpretation featured in this book succeeds without any change in the theory It involves one radical step the reinterpretation of an assumption that was virtually never questioned before the traditional eigenvalue link between theory and observation is replaced by a q expectation link Objective properties are given by q expectations of products of quantum fields and what is computable from these Averaging over macroscopic spacetime regions produces macroscopic quantities with negligible uncertainty and leads to classical physics Reflects the actual practice of quantum physics Models the quantum classical interface through coherent spaces Interprets both quantum mechanics and quantum field theory Eliminates probability and measurement from the foundations Proposes a novel solution of the measurement Building Blocks Of Nuclear Structure, The - 4th International Spring Seminar On Nuclear Physics Aldo problem Covello,1993-05-31 Held in May 1992 in Italy the 4th International Spring Seminar on Nuclear Physics focused on recent developments which enhanced our understanding of the role of the various degrees of freedom which come into play in the nucleus Consisting of four sessions the first three sessions dealt with both theoretical and experimental issues centering on quarks and meson degrees of freedom single particle degrees of freedom and collective degrees of freedom The fourth session discussed several important contributions that nuclear structure physics has made to the other research fields

Attosecond Molecular Dynamics Marc J J Vrakking, Franck Lepine, 2018-08-31 Attosecond science is a new and rapidly developing research area in which molecular dynamics are studied at the timescale of a few attoseconds Within the past decade attosecond pump probe spectroscopy has emerged as a powerful experimental technique that permits electron dynamics to be followed on their natural timescales With the development of this technology physical chemists have been

able to observe and control molecular dynamics on attosecond timescales From these observations it has been suggested that attosecond to few femtosecond timescale charge migration may induce what has been called post Born Oppenheimer dynamics where the nuclei respond to rapidly time dependent force fields resulting from transient localization of the electrons These real time observations have spurred exciting new advances in the theoretical work to both explain and predict these novel dynamics This book presents an overview of current theoretical work relevant to attosecond science written by theoreticians who are presently at the forefront of its development It is a valuable reference work for anyone working in the field of attosecond science as well as those studying the subject *Group Theoretical Methods in Physics M.* A. Markov, A. E. Shabad, 1985 Nonequilibrium Physics at Short Time Scales Klaus Morawetz, 2013-03-09 This book is the result of the many discussions and collaborations that de veloped from the seven previous workshops held on this topic This ongoing series of interdisciplinary workshops provided an opportunity for the presentation and exchange of results describing nonequilibrium phenomena at short time scales The important questions concern the correlation and memory ef fects in dense interacting systems currently under study in various areas of physics Experiments on very short time scales are especially characterized by the strong correlations in systems far from equilibrium and by their non linear dynamics In this regard conventionally applied theoretical techniques are critically reviewed and new theoretical concepts are discussed Possible signals of nonequilibrium effects are extracted from experiments using power ful techniques and skills The exchange of views and techniques from different areas of physics helped to stimulate such developments. The impressive success of experiments using short laser pulses to probe the properties of matter as well as of the new methods of analysis of the early phases of heavy ion reactions initiated a review of the available many body theoretical methods These statistical methods describing strong nonequilib rium situations were known at least partially for a long time However recent developments in computing power have provided the possibility of accurately comparing ab initio and approximate methods Approaches to Quantum Liquids in Confined Geometries Eckhard Krotscheck, Jes£s Navarro, 2002 This volume assembles review articles that present the status of frontline research in this field in a manner that makes the material accessible to the educated but non specialist reader The articles focus on the many body aspects of the theory of quantum liquids in confined geometry Research is in the very satisfactory situation where several accurate approaches are available that allow one to describe these systems in a quantitative manner without modelling uncertainty and uncontrolled assumptions For example dynamic situations of direct experimental relevance can be modelled with high accuracy *Understanding The Variety Of* Nuclear Excitations - Proceedings Of The 3rd International Spring Seminar On Nuclear Physics Aldo Covello, 1991-03-15 The primary emphasis of the Seminar is on the modes of excitation in both spherical and deformed nuclei Several topics at the forefront of current research in nuclear structure are covered by leading physicists. The main themes are Single particle and Collective Degrees of Freedom in Low energy Modes of Excitation The Nature of High spin States in Deformed and Spherical

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