

1. Record Nr.	UNINA9910993973603321
Titolo	Complex quantum systems : analysis of large Coulomb systems / / editor: Heinz Siedentop
Pubbl/distr/stampa	[Hackensack], NJ, : World Scientific, c2013 New Jersey : , : World Scientific, , [2013] 2013
ISBN	9789814460156 981446015X 9789814460149
Edizione	[1st ed.]
Descrizione fisica	1 online resource (303 pages)
Collana	Lecture notes series, , 1793-0758 ; ; v. 24
Altri autori (Persone)	SiedentopHeinz
Disciplina	530.12
Soggetti	Quantum statistics Quantum electrodynamics - Mathematics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references.
Nota di contenuto	Intro -- CONTENTS -- Foreword -- Preface -- Stability of Matter Rafael D. Benguria and Benjamn A. Loewe -- 1. Introduction: The stability of quantum systems: A historical overview -- 2. Stability of Matter: The classical proof of Lieb and Thirring -- 2.1. Stability of the hydrogen atom in non-relativistic quantum mechanics -- 2.2. Stability of a system of N electrons in non-relativistic quantum mechanics -- 2.3. Stability of a many particle system via Thomas-Fermi theory -- 2.4. Bibliographical remarks -- 3. Lieb-Thirring Inequalities -- 3.1. Use of commutation methods to prove the Lieb-Thirring inequality for $\mu = 3/2$ in dimension 1 -- 3.2. The Eden-Foias bound ([46]) -- 3.3. Bibliographical remarks -- 4. Electrostatic Inequalities -- 5. The Maximum Number of Electrons an Atom Can Bind -- 5.1. The maximum number of electrons for a one center case in the Thomas-Fermi model -- 5.2. Bound on $N_c(Z)$ for the TFW model in the atomic case -- 6. The Stability of Matter for a Relativistic Toy Model -- 6.1. Bibliographical remarks -- 7. A New Lieb-Oxford Bound with Gradient Corrections -- Acknowledgments -- Appendix: A Short History of the Atom -- References -- Mathematical Density and Density Matrix

Functional Theory (DFT and DMFT) Volker Bach -- 1. Introduction -- 2. Exchange Correlation and LDA -- 3. Kinetic Energy and Lieb-Thirring Inequality -- 4. Thomas-Fermi Theory and Stability of Matter -- 5. Hartree-Fock Theory -- 6. Correlation Estimate Improving the Lieb-Oxford Inequality -- 7. Accuracy of the Hartree-Fock Approximation for Large Neutral Atoms -- 8. N-Representability -- Acknowledgments -- References -- On the Dynamics of a Fermi Gas in a Random Medium with Dynamical Hartree-Fock Interactions Thomas Chen -- 1. Introduction -- Acknowledgment -- 2. Fermi Gas in a Random Medium -- 2.1. Statement of the main results. 2.2. Boltzmann limit of the momentum distribution function -- 2.3. Outline of the proof -- 2.4. Feynman graph expansion -- 2.5. Classification of graphs -- 2.6. Discussion of the result -- 3. Persistence of Quasifreeness in the Boltzmann Limit -- 3.1. Outline of the proof of Theorem 3.1 -- 3.1.1. Completely disconnected graphs -- 3.1.2. Non-disconnected graphs -- 4. Fermi Gas with Dynamical Hartree-Fock Interactions -- 4.1. Statement of main results -- 4.1.1. The regime C_2 -- 4.1.2. The regime $= o()$ -- 4.1.3. The regime $t = T/2$ and $= O(1)$ -- References -- On the Minimization of Hamiltonians over Pure Gaussian States Jan Dereziński, Marcin Napiórkowski, and Jan Philip Solovej -- 1. Introduction -- Acknowledgments -- 2. Preliminaries -- 2.1. 2nd quantization -- 2.2. Wick quantization -- 2.3. Bogoliubov transformations -- 2.4. Pure Gaussian states -- 3. Main Result -- References -- Variational Approach to Electronic Structure Calculations on Second-Order Reduced Density Matrices and the N-Representability Problem Maho Nakata, Mitsuhiro Fukuda, and Katsuki Fujisawa -- 1. Introduction -- 2. The Reduced-Density-Matrix Method -- 2.1. Pure states and ensemble states -- 2.2. The first-order and second-order reduced density matrices -- 2.2.1. Coordinate representation -- 2.2.2. Second-quantized representation -- 2.2.3. Equivalence between the coordinate and second-quantized representations -- 2.2.4. Some properties of 1- and 2-RDMs -- 2.3. Solving the ground state problem using 1- and 2-RDMs -- 2.4. The N-representability problem and the N-representability conditions -- 2.5. On the complete N-representability conditions -- 2.6. Formulating the variational problem and its geometrical representation -- 2.7. Some of the known necessary N-representability conditions -- 2.8. The reduced-density-matrix method -- 2.9. Interpreting the conditions. 3. Formulating the RDM Problem as a Semidefinite Program and its Solution Using the Interior-Point Method -- 3.1. Semidefinite program -- 3.2. Formulation of the RDM problem as an SDP -- 3.3. Theoretical computational complexity of the primal-dual interior-point method -- 4. Some Historical Remarks -- 5. Numerical Results for the RDM Method -- 5.1. New numerical results for larger systems -- 5.2. Summary of the numerical experiments -- 6. Concluding Remarks -- Acknowledgments -- References -- Fermionic Quantum Many-Body Systems: A Quantum Information Approach Christina V. Kraus -- 1. Introduction -- 2. Pairing in Fermionic Systems: A Quantum Information Perspective -- 2.1. Motivation -- 2.2. Pairing theory -- 2.3. Detection and quantification of pairing -- 2.3.1. Detection of pairing -- 2.4. Examples: Fermionic Gaussian states and number-conserving states -- 2.4.1. Pairing of Gaussian states -- 2.4.2. Pairing of number-conserving states -- 2.5. Pairing as a resource -- 3. Fermionic Projected Entangled Pair State -- 3.1. A review of the PEPS-construction -- 3.2. Construction of fPEPS -- 3.3. Relation between fPEPS and PEPS -- 3.4. Examples -- 4. Conclusion and Outlook -- Acknowledgments -- References -- Hydrogen-Like Atoms in

Relativistic QED Martin Konenbergh, Oliver Matte, and Edgardo Stockmeyer -- 1. Introduction -- 2. Definition of the Models -- 2.1. Operators in Fock-space -- 2.2. Interaction term -- 2.3. The semi-relativistic Pauli-Fierz and no-pair Hamiltonians -- 2.4. How to deal with the non-local terms -- 3. Self-Adjointness -- 3.1. Diamagnetic inequalities in QED -- 3.2. Semi-boundedness -- 4. Bounds on the Ionization Energy -- 5. Exponential Localization -- 5.1. A general strategy to prove the localization of spectral subspaces -- 5.2. Choice of the comparison operator Y -- 5.3. Conjugation of Y with exponential weights. 6. Existence of Ground States with Mass -- 6.1. Operators with photon mass -- 6.2. Discretization of the photon momenta -- 6.3. Comparison of operators with different coupling functions -- 6.4. Higher order estimates and their consequences -- 6.5. Continuity of the ionization thresholds and ground state energies -- 6.6. Proofs of the existence of ground states with mass -- 7. Infra-Red Bounds -- 7.1. The gauge transformed operator -- 7.2. Soft photon bound for the semi-relativistic Pauli-Fierz operator -- 8. Existence of Ground States -- 8.1. Ground states without photon mass -- 8.2. Ground state degeneracy -- 9. Commutator Estimates -- 9.1. Basic estimates -- 9.2. Commuting projections with the field energy -- 9.3. Double commutators -- Acknowledgments -- References.

Sommario/riassunto

This volume is based on lectures given during the program Complex Quantum Systems held at the National University of Singapore's Institute for Mathematical Sciences from 17 February to 27 March 2010. It guides the reader through two introductory expositions on large Coulomb systems to five of the most important developments in the field: derivation of mean field equations, derivation of effective Hamiltonians, alternative high precision methods in quantum chemistry, modern many body methods originating from quantum information, and - the most complex - semirelativistic quantum electrodynamics.
