

1. Record Nr.	UNINA9910140440903321
Titolo	Quantum information and computation for chemistry . Volume 154 Advances in chemical physics // edited by Sabre Kais, Stuart A. Rice, Aaron R. Dinner
Pubbl/distr/stampa	Hoboken, New Jersey : , : Wiley, , 2014 ©2014
ISBN	1-118-74263-X 1-118-74260-5 1-118-74258-3
Descrizione fisica	1 online resource (673 p.)
Collana	Advances in Chemical Physics ; ; Volume 154
Classificazione	VE 2300 UA 1024 VC 6100
Altri autori (Persone)	KaisSabre RiceStuart A DinnerAaron R
Disciplina	541.3
Soggetti	Chemistry, Physical and theoretical
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 at the end of each chapters and indexes.
Nota di contenuto	Quantum Information and Computation for Chemistry; Contributors to Volume 154; Foreword; Preface to The Series; Contents; Introduction to Quantum Information and Computation for Chemistry; I. Introduction; A. Qubits and Gates; B. Circuits and Algorithms; C. Teleportation; II. Quantum Simulation; A. Introduction; B. Phase Estimation Algorithm; 1. General Formulation; 2. Implementation of Unitary Transformation U; 3. Group Leaders Optimization Algorithm; 4. Numerical Example; 5. Simulation of the Water Molecule; III. Algorithm for Solving Linear Systems $Ax = b$; A. General Formulation B. Numerical Example IV. Adiabatic Quantum Computing; A. Hamiltonians of n-Particle Systems; B. The Model of Adiabatic Computation; C. Hamiltonian Gadgets; V. Topological Quantum Computing; A. Anyons; B. Non-Abelian Braid Groups; C. Topological Phase of Matter; D. Quantum Computation Using Anyons; VI.

Entanglement; VII. Decoherence; VIII. Major Challenges and Opportunities; References; Back to The Future: A Roadmap for Quantum Simulation from Vintage Quantum Chemistry; I. Introduction; II. Quantum Computing; A. Phase Estimation; B. Time Evolution and the Cartan Decomposition
III. Quantum Chemistry: The CI Method A. Second Quantization: Direct Mapping; B. FCI: Compact Mapping; IV. A Selection of Historical Calculations in Quantum Chemistry; A. The 1930's and 1940's; B. The 1950's; C. The 1960's; V. Boys's 1950 Calculation for Be; VI. Conclusions; References; Introduction to Quantum Algorithms for Physics and Chemistry; I. Introduction; A. Quantum Computational Complexity and Chemistry; 1. An Exponential Wall for Many-Body Problems; 2. Computational Complexity of Quantum Simulation; B. Basic Quantum Algorithms for Digital Quantum Simulation; 1. Quantum Fourier Transform
2. Phase Estimation Algorithm II. Digital Quantum Simulation; A. Overview; B. Simulation of Time Evolution; 1. Suzuki-Trotter Formulas; 2. First-Quantized Representation; 3. Second-Quantized Representation; 4. Open-System Dynamics; C. State Preparation; 1. Preparing Ground States; 2. Preparing Thermal States Using Quantum Metropolis; 3. Preparing Thermal States with Perturbative Updates; D. Algorithmic Quantum Cooling; 1. Basic Idea of the Quantum Cooling Method; 2. Connection with Heat-Bath Algorithmic Cooling; III. Special Topics; A. Adiabatic Nondestructive Measurements
B. TDDFT and Quantum Simulation IV. Conclusion and Outlook; References; Quantum Computing Approach to Nonrelativistic and Relativistic Molecular Energy Calculations; I. Overview; II. Quantum Computing Background; A. Quantum Fourier Transform; B. Semiclassical Approach to Quantum Fourier Transform; C. Phase Estimation Algorithm; D. Iterative Phase Estimation Algorithm; III. Quantum Full Configuration Interaction Method; A. Mapping of Quantum Chemical Wave Functions onto Quantum Register; B. Initial States for the Algorithm; 1. Adiabatic State Preparation; C. Controlled "Time Propagation"
1. Decomposition of Unitary Propagator to Elementary Quantum Gates

Sommario/riassunto

Examines the intersection of quantum information and chemical physics The Advances in Chemical Physics series is dedicated to reviewing new and emerging topics as well as the latest developments in traditional areas of study in the field of chemical physics. Each volume features detailed comprehensive analyses coupled with individual points of view that integrate the many disciplines of science that are needed for a full understanding of chemical physics. This volume of the series explores the latest research findings, applications, and new research paths from the quantum information.
