

Efficient Mean-Field Simulation of Quantum Circuits Inspired by the Many-Electron Problem

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Classical simulations can provide the exact wave function of quantum circuits (QCs)^{1–3}, but are currently limited to ~ 50 qubits^{1,4} due to their memory and computational cost, which scale exponentially with qubit number. As quantum hardware advances toward hundreds of interacting qubits⁵, developing reliable schemes for approximate QC simulations has become a priority. Here we show efficient simulations of QCs with a method inspired by density functional theory (DFT), a widely used approach to study many-electron systems. We demonstrate accurate simulations of various QCs with universal gate sets, reaching up to a billion qubits in size, using only laptop calculations. Our simulations can predict marginal single-qubit probabilities (SQPs) with over 90% accuracy, using memory and computational resources linear in qubit number despite the formal exponential cost of SQPs. We achieve these results by adopting a mean-field description of QCs, and formulating optimal single- and two-qubit gate functionals – analogs of exchange-correlation functionals in DFT⁶ – to evolve the SQPs without computing the QC wave function. Our findings pave the way for accurate simulations of large QCs and provide a blueprint to adapt electronic structure methods to QC simulations.

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Lectures on the Many-electron Problem Robert Brout, Peter A. Carruthers, 1963 **The Many-electron Problem** K. S. Viswanathan, 1966 **Many-Electron Approaches in Physics, Chemistry and Mathematics** Volker Bach, Luigi Delle Site, 2014-07-01 This book provides a broad description of the development and computational application of many electron approaches from a multidisciplinary perspective In the context of studying many electron systems Computer Science Chemistry Mathematics and Physics are all intimately interconnected However beyond a handful of communities working at the interface between these disciplines there is still a marked separation of subjects This book seeks to offer a common platform for possible exchanges between the various fields and to introduce the reader to perspectives for potential further developments across the disciplines The rapid advances of modern technology will inevitably require substantial improvements in the approaches currently used which will in turn make exchanges between disciplines indispensable In essence this book is one of the very first attempts at an interdisciplinary approach to the many electron problem Solving the Many Electron Problem with Quantum Monte-Carlo Methods Alan John James, 1996 The Many-electron Problem [by] K.S. Viswanathan K. S. Viswanathan, 1966 **Some Approaches to the Many-electron Problem in Chemistry** John William Kenney, 1979 The many electron problem D. M. Drew, 1964 **The Symmetric Group in Quantum Chemistry** R. Pauncz, 2018-05-04 This is the first book to provide comprehensive treatment of the use of the symmetric group in quantum chemical structures of atoms molecules and solids It begins with the conventional Slater determinant approach and proceeds to the basics of the symmetric group and the construction of spin eigenfunctions The heart of the book is in the chapter dealing with spin free quantum chemistry showing the great interpretation value of this method The last three chapters include the unitary group approach the symmetric group approach and the spin coupled valence bond method An extensive bibliography concludes the book *Theoretical Solid State Physics* Albert Haug, 2016-04-20 *Theoretical Solid State Physics* Volume 1 focuses on the study of solid state physics The volume first takes a look at the basic concepts and structures of solid state physics including potential energies of solids concept and classification of solids and crystal structure The book then explains single electron approximation wherein the methods for calculating energy bands electron in the field of crystal atoms laws of motion of the electrons in solids and electron statistics are discussed The text describes general forms of solutions and relationships including collective electron interactions Hartree Fock and Heitler London methods and electron electron scattering The volume also reviews the magnetic properties of solids Paramagnetism and diamagnetism of free electrons solids and atoms behavior of electrons in a magnetic field and basic concepts of magnetism are discussed The book also considers the dielectric properties of solids and dynamics of crystal lattices The volume is a dependable source of data for readers interested in solid state physics **Introduction to the Field Theoretical Approach to the Many-electron Problem** Lars Hedin (Physician.), Stig Lundqvist, 1960 *Lectures on the Many-electron*

Problem [by] R. Brout [and] P. Carruthers R. Brout, Peter Ambler Carruthers, 1963 *An Algebraic Approach to the Many-Electron Problem* Jaroslav Zamastil, Tereza Uhlířová, 2025-06-08 This book presents an algebraic approach to the coupled cluster method for many electron systems pioneered by Josef Paldus Using field methods along with an algebraic rather than diagrammatic approach facilitates a way of deriving the coupled cluster method which is readily understandable at the graduate level The book begins with the notion of the quantized electron field and shows how the N electron Hamiltonian can be expressed in its language This is followed by introduction of the Fermi vacuum and derivation of the Hartree Fock equations along with conditions for stability of their solutions Following this groundwork the book discusses a method of configuration interaction to account for dynamical correlations between electrons pointing out the size extensivity problem and showing how this problem is solved with the coupled cluster approach This is followed by derivation of the coupled cluster equations in spin orbital form Finally the book explores practical aspects showing how one may take advantage of permutational and spin symmetries and how to solve coupled cluster equations illustrated by the Hubbard model of benzene the simplest quasi realistic model of electron correlation *Introduction to Modern Inorganic Chemistry, 6th edition* R.A. Mackay, 2017-12-21 This popular and comprehensive textbook provides all the basic information on inorganic chemistry that undergraduates need to know For this sixth edition the contents have undergone a complete revision to reflect progress in areas of research new and modified techniques and their applications and use of software packages Introduction to Modern Inorganic Chemistry begins by explaining the electronic structure and properties of atoms then describes the principles of bonding in diatomic and polyatomic covalent molecules the solid state and solution chemistry Further on in the book the general properties of the periodic table are studied along with specific elements and groups such as hydrogen the s elements the lanthanides the actinides the transition metals and the p block Simple and advanced examples are mixed throughout to increase the depth of students understanding This edition has a completely new layout including revised artwork case study boxes technical notes and examples All of the problems have been revised and extended and include notes to assist with approaches and solutions It is an excellent tool to help students see how inorganic chemistry applies to medicine the environment and biological topics **The Variation Principle and the Many Electron Problem** George Sidney Handler, 1955 **New Advances in Semiconductors** Alberto Adriano Cavalheiro, 2022-06-15 New Advances in Semiconductors brings together contributions from important researchers around the world on semiconductor materials and their applications It includes seven chapters in two sections Calculations and Simulations in Semiconductors and Semiconductor Materials The world will emerge different after the social and economic reorganizations caused by the COVID 19 pandemic and will be even more dependent on semiconductors than ever before New Advances in Semiconductors is a book that brings together the contributions of important researchers around the world and is able to give an idea about the different characteristics of semiconductor materials and their applications There is a section dedicated to theory calculations

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