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Descrizione fisica	1 online resource (XIII, 494 p. 1 illus.)
Collana	Undergraduate Lecture Notes in Physics, , 2192-4791
Disciplina	530.12
Soggetti	Quantum theory Physics Atomic structure Molecular structure Quantum Physics Numerical and Computational Physics, Simulation Atomic/Molecular Structure and Spectra
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Part I Scientific programming: an introduction for physicists: Numbers and precision -- Fortran -- Python -- Part II Numerical methods for quantum physics: Finding roots -- Differentiation and initial value problems -- Numerical integration -- The eigenvalue problem -- The Fourier transform -- PART III Solving the Schrödinger equation: One dimension -- Higher dimensions and basic techniques -- Time propagation -- Central potentials -- Multi-electron systems -- Exercises.
Sommario/riassunto	Quantum mechanics undergraduate courses mostly focus on systems with known analytical solutions; the finite well, simple Harmonic, and spherical potentials. However, most problems in quantum mechanics cannot be solved analytically. This textbook introduces the numerical techniques required to tackle problems in quantum mechanics, providing numerous examples en route. No programming knowledge is required – an introduction to both Fortran and Python is included, with code examples throughout. With a hands-on approach, numerical techniques covered in this book include differentiation and integration,

ordinary and differential equations, linear algebra, and the Fourier transform. By completion of this book, the reader will be armed to solve the Schrodinger equation for arbitrarily complex potentials, and for single and multi-electron systems.