



Chapter 015, Density Functional Theory

Yehuda Band

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NOTE: This is a single chapter excerpted from the book *Quantum Mechanics with Applications to Nanotechnology and Information Science*, made available for individual purchase. Additional chapters, as well as the entire book, may be purchased separately.

Quantum mechanics transcends and supplants classical mechanics at the atomic and subatomic levels. It provides the underlying framework for many subfields of physics, chemistry and materials science, including condensed matter physics, atomic physics, molecular physics, quantum chemistry, particle physics, and nuclear physics. It is the only way we can understand the structure of materials, from the semiconductors in our computers to the metal in our automobiles. It is also the scaffolding supporting much of nanoscience and nanotechnology. The purpose of this book is to present the fundamentals of quantum theory within a modern perspective, with emphasis on applications to nanoscience and nanotechnology, and information-technology. As the frontiers of science have advanced, the sort of curriculum adequate for students in the sciences and engineering twenty years ago is no longer satisfactory today. Hence, the emphasis on new topics that are not included in older reference texts, such as quantum information theory, decoherence and dissipation, and on applications to nanotechnology, including quantum dots, wires and wells.

Key Features

- This book provides a novel approach to Quantum Mechanics whilst also giving readers the requisite background and training for the scientists and engineers of the 21st Century who need to come to grips with quantum phenomena.
- The fundamentals of quantum theory are provided within a modern perspective, with emphasis on applications to nanoscience and nanotechnology, and information-technology.

Benefits

- Older books on quantum mechanics do not contain the amalgam of ideas, concepts and tools necessary to prepare engineers and scientists to deal with the new facets of quantum mechanics and their application to quantum information science and nanotechnology.
- As the frontiers of science have advanced, the sort of curriculum adequate for students in the sciences and engineering twenty years ago is no longer satisfactory today.
- There are many excellent quantum mechanics books available, but none have the emphasis on nanotechnology and quantum information science that this book has.

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