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Nota di contenuto	1. Introduction -- 2. Basic Formalism for Stationary Non-Relativistic Systems -- 2.1 The Hohenberg-Kohn Theorem -- 2.2 Degenerate Groundstates -- 2.3 v-Representability and Related Questions -- 2.4 Fractional Particle Number, Chemical Potential, and Derivative Discontinuities -- 3. Extensions -- 3.1 Spin-Polarised Systems -- 3.2 Finite Temperature Ensembles -- 3.3 Multicomponent Systems -- 3.4 Hartree-Fock Limit -- 3.5 Excited States -- 3.6 Density Matrix Functionals -- 3.7 Momentum Space -- 3.8 Bose Systems -- 3.9 Superconducting Systems -- 4. The Kohn-Sham Scheme -- 4.1 The Basic Kohn-Sham Equations -- 4.2 Degenerate Kohn-Sham Groundstates and the Question of v-Representability -- 4.3 Spin-Polarised Systems -- 4.4 Fractional Occupation, Janak’s Theorem, and

the Slater Transition State -- 4.5 Excited States: The Kohn-Sham Scheme for Ensembles -- 4.6 Schrödinger Equation for the Square Root of the Groundstate Density -- 4.7 Hellmann-Feynman, Virial, and Scaling Properties of Density Functionals -- 4.8 Single-Particle Equations for Superconductors: A Generalized Bogoliubov-deGennes Scheme -- 5. Explicit Functionals I: Kinetic and Exchange Energy Functionals Derived from the One-Particle Density Matrix -- 5.1 Density-Gradient Expansions from Semiclassical Expansions: A Survey -- 5.2 The Kirzhnits Method -- 5.3 The Wigner-Kirkwood Approach and Partial Resummation of the Gradient Expansion -- 5.4 Empirical Convergence Studies of the Gradient Expansion -- 5.5 Original von Weizsäcker Functional Versus Gradient Expansion -- 5.6 Padé Approximants and Other Parametrisations -- 5.7 Phase-Space Approach Based on Local Thermodynamics -- 5.8 The Classical Density Functional Models of Thomas, Fermi, Dirac, and von Weizsäcker -- 6. Many-Body Perturbation Theory -- 6.1 Diagrammatic Approach to the InhomogeneousElectron Gas -- 6.2 The Exchange-Correlation Functional Expressed in Terms of the Irreducible Self-Energy -- 6.3 The Band Gap in Insulators and Semiconductors -- 6.4 The Fermi Surface in Metals -- 6.5 The Homogeneous Electron Gas -- 7. Explicit Functionals II: The Local Density Approximation and Beyond -- 7.1 The Local Density Approximation -- 7.2 Discussion of the Local Density Approximation -- 7.3 Nonlocal Density Schemes -- 7.4 Self-Interaction Corrections -- 7.5 Wave Vector Analysis -- 7.6 Gradient Corrections -- 7.7 Kohn-Sham Results for Atoms and Molecules -- 8. Density Functional Theory of Relativistic Systems -- 8.1 Introduction -- 8.2 Existence Theorems -- 8.3 Explicit Functionals I: The Relativistic Kirzhnits Expansion -- 8.4 The Homogeneous Relativistic Electron Gas -- 8.5 Explicit Functionals II: The Local Density Approximation -- 8.6 Remarks and Applications -- A. Definition of Density Matrices, Green's Functions, and Correlation Functions -- B. Compilation of Literature on Atomic and Molecular Kohn-Sham Results -- References.

Sommario/riassunto

Density Functional Theory is a rapidly developing branch of many-particle physics that has found applications in atomic, molecular, solid-state and nuclear physics. This book describes the conceptual framework of density functional theory and discusses in detail the derivation of explicit functionals from first principles as well as their application to Coulomb systems. Both non-relativistic and relativistic systems are treated. The connection of density functional theory with other many-body methods is highlighted. The presentation is self-contained; the book is, thus, well suited for a graduate course on density functional theory.