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Its Applications in Orbital-Free DFT Simulations; 1. From the Hohenberg-Kohn Theory to the Kohn-Sham Equations Y. A. Wang & P. Xiang; 1.1. Introduction; 1.2. Routes to the Kohn-Sham equations; 1.3. A paradox and its resolution; 1.3.1. The Wang paradox; 1.3.2. The Wang-Parr resolution; 1.4. Direct inclusion of the constraints; 1.5. Functional derivative of the kinetic-energy density functional; 1.6. Conclusions; Acknowledgement; References
2. Accurate Computation of the Non-Interacting Kinetic Energy from Electron Densities F. A. Bulat & W. Yang2.1. Introduction; 2.2. Theory; 2.2.1. Direct optimization method for the Kohn-Sham kinetic energy functional Ts and the exact exchange-correlation potential vxc; 2.2.2. Exchange vx and correlation vc components of the exchange-correlation potential vxc; 2.3. Regularization of the WY functional; 2.4. Results and discussion; 2.4.1. Exchange-correlation vxc(r) potentials; 2.4.2. Kohn-Sham kinetic energy; 2.4.3. Exchange vx(r) and correlation vc(r) potentials; 2.5. Conclusions
AcknowledgementsReferences; 3. The Single-Particle Kinetic Energy of Many-Fermion Systems: Transcending the Thomas-Fermi plus Von Weizs acker Method G. G. N. Angilella & N. H. March; 3.1. Background and outline; 3.2. Fermions in surface regimes: nuclei and simple liquid metals; 3.2.1. The nucleon surface density; 3.2.2. Brief background on surface energies; 3.2.2.1. Nucleon surface energies; 3.2.2.2. Application to a liquid metal planar surface; 3.3. Variational principle for the TF plus von Weizsacker (TFvW) method; 3.4. Differential virial theorem and the Dirac density matrix
3.4.1. Relation of the exact DVT to the semiclassical Thomas-Fermi method3.5. Perturbative expansion of Dirac density matrix (r, r') in powers of the given one-body potential V (r); 3.5.1. Stoddart-March series for the kinetic energy density t(r) in three dimensions; 3.6. Complete DFT for harmonically confined Fermions in D dimensions, for an arbitrary number of closed shells; 3.6.1. Current experimental focus on many Fermions that are harmonically confined; 3.6.2. Differential equation for Fermion density
3.6.3. Kinetic energy density functional t[ ] for arbitrary number of Fermions moving independently in one-dimensional harmonic oscillator potential3.6.4. Summary of complete DFT for many closed shells of Fermions which are (isotropically) harmonically confined in D dimensions; 3.7. The Pauli potential in relation to the functional derivative of the single-particle kinetic energy density; 3.7.1. Relation to the differential virial theorem; 3.7.2. Example of harmonic confinement; 3.8. Non-local potential theory: V (r) V (r, r')
3.8.1. Fine-tuning of Hartree-Fock (HF) density for spherical atoms like neon

Sommario/riassunto

This is a comprehensive overview of state-of-the-art computational methods based on orbital-free formulation of density functional theory completed by the most recent developments concerning the exact properties, approximations, and interpretations of the relevant quantities in density functional theory.The book is a compilation of contributions stemming from a series of workshops which had been taking place since 2002. It not only chronicles many of the latest developments but also summarises some of the more significant ones. The chapters are mainly reviews of sub-domains but also include or