

1. Record Nr.	UNINA9910491030503321
Autore	Gallo Paola
Titolo	Physics of liquid matter / / Paola Gallo and Mauro Rovere
Pubbl/distr/stampa	Cham, Switzerland : , : Springer, , [2021] ©2021
ISBN	3-030-68349-4
Descrizione fisica	1 online resource (338 pages)
Collana	Soft and Biological Matter
Disciplina	632.05
Soggetti	Fluid dynamics Hydrodynamics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes index.
Nota di contenuto	Intro -- Preface -- Contents -- Acronyms -- 1 An Introduction to the Liquid State of Matter -- 1.1 Liquid State of Matter -- 1.1.1 Examples of Phase Diagram of Pure Substances: CO ₂ and Water -- 1.1.2 Phase Diagram of Binary Mixtures -- 1.2 Structure and Dynamics of Liquids: Experiments and Correlation Functions -- 1.3 Microscopic Models for Liquids -- 1.3.1 Classical Approximation -- 1.3.2 Different Models -- 1.4 Potential Energy Landscape -- 1.5 Approximate Theories and Computer Simulation -- 1.6 Water and Hydrogen Bond -- 1.7 Metastable States and Disordered Solid Matter -- 1.8 Soft Matter -- 1.8.1 Colloids -- 1.8.2 Biomolecules -- References -- 2 Thermodynamics and Statistical Mechanics of Fluid States -- 2.1 Extensive and Intensive Functions -- 2.2 Energy and Entropy -- 2.3 Gibbs-Duhem Relation -- 2.4 Equilibrium Conditions -- 2.5 Equilibrium Conditions and Intensive Quantities -- 2.6 Macroscopic Response Functions and Stability Conditions -- 2.7 Legendre Transforms and Thermodynamic Potentials -- 2.7.1 Helmholtz Free Energy -- 2.7.2 Gibbs Free Energy -- 2.7.3 Enthalpy -- 2.7.4 Grand Canonical Potential -- 2.7.5 Tabulated Thermodynamic Potentials -- 2.8 Stability Conditions for Thermodynamic Potentials -- 2.9 Coexistence and Phase Transitions -- 2.10 Phase Transitions and Their Classifications -- 2.11 Van der Waals Equation -- 2.12 General Form of the Van der Waals Equation and Corresponding States -- 2.13 Critical

Behaviour of the Van der Waals Equation -- 2.14 Ensembles in Statistical Mechanics -- 2.14.1 Microcanonical Ensemble -- 2.14.2 Canonical Ensemble -- 2.14.3 Grand Canonical Ensemble -- 2.14.4 Isobaric-Isothermal Ensemble -- 2.15 Fluctuations and Thermodynamics -- References -- 3 Microscopic Forces and Structure of Liquids -- 3.1 Force Field for Atoms in Liquids -- 3.2 Local Structure of a Liquid.

3.3 Distribution Functions in the Canonical Ensemble -- 3.4 Relation of the RDF with Thermodynamics -- 3.4.1 Energy -- 3.4.2 Pressure from the Virial -- 3.5 Distribution Functions in the Grand Canonical Ensemble -- 3.6 Hierarchical Equations -- 3.7 Qualitative Behaviour of the Radial Distribution Function -- 3.8 Experimental Determination of the Structure of Liquids -- 3.9 Neutron Scattering on Liquids -- 3.10 Static Limit and the Structure of Liquid -- 3.11 The Static Structure Factor -- 3.12 The Structure Factor and the RDF of Liquid Argon -- 3.13 The Structure Factor Close to a Critical Point -- 3.14 Structure of Multicomponent Liquids -- 3.14.1 Partial Structure Factor of Multicomponent Liquids -- 3.14.2 Isotopic Substitution -- 3.14.3 An Example: Molten Salts -- 3.15 Structure of Molecular Liquids -- 3.15.1 Structure of Liquid Water -- References -- 4 Theoretical Studies of the Structure of Liquids -- 4.1 Virial Expansion in the Canonical Ensemble -- 4.1.1 From Hard Spheres to the Van der Waals Equation -- 4.2 The Mean Force Potential -- 4.3 Kirkwood Approximation -- 4.4 Radial Distribution Function from the Excess Free Energy -- 4.5 Density Distributions from the Grand Partition Function -- 4.6 Grand Potential as Generating Functional -- 4.7 Classical Density Functional Theory -- 4.7.1 Equilibrium Conditions -- 4.7.2 The Ornstein-Zernike Equation -- 4.7.3 The Ornstein-Zernike Equation in k-Space -- 4.7.4 Free Energy Calculation -- 4.7.5 Expansion from the Homogeneous System -- 4.8 Closure Relations from the Density Functional Theory -- 4.9 An Exact Equation for the $g(r)$ -- 4.10 HNC and Percus-Yevick Approximations -- 4.10.1 RPA and MSA -- 4.11 Properties of the Hard Sphere Fluid -- 4.12 Equation of State and Liquid-Solid Transition of Hard Spheres -- 4.13 Percus-Yevick for the Hard Sphere Fluid.

4.14 Equation of State and Thermodynamic Inconsistency -- 4.15 Routes to Consistency: Modified HNC and Reference HNC -- 4.16 Perturbation Theories: Optimized RPA -- 4.17 Models for Colloids -- References -- 5 Methods of Computer Simulation -- 5.1 Molecular Dynamics Methods -- 5.1.1 Molecular Dynamics and Statistical Mechanics -- 5.1.2 Algorithms for the Time Evolution -- 5.1.3 Predictor/Corrector -- 5.1.4 Verlet Algorithms -- Velocity Verlet -- Leapfrog -- 5.1.5 Calculation of the Forces -- 5.1.6 Initial Configuration -- 5.1.7 Temperature in the Microcanonical Ensemble -- 5.1.8 Equilibration Procedure -- 5.1.9 Thermodynamic and Structure -- 5.1.10 Long-Range Corrections -- 5.1.11 Ewald Method -- 5.2 Monte Carlo Simulation -- 5.2.1 Monte Carlo Integration and Importance Sampling -- 5.2.2 Integrals in Statistical Mechanics -- 5.2.3 Importance Sampling in Statistical Mechanics -- 5.2.4 Markov Processes -- 5.2.5 Ergodicity and Detailed Balance -- 5.2.6 Metropolis Method -- 5.2.7 Averaging on Monte Carlo Steps -- 5.2.8 MC Sampling in Other Ensembles -- Isobaric-Isothermal MC -- Grand Canonical MC -- 5.2.9 MC in the Gibbs Ensemble -- 5.3 MD in Different Ensembles -- 5.3.1 Controlling the Temperature: MD in the Canonical Ensemble -- The Nose Method -- Hoover Equations -- 5.3.2 Pressure Control -- 5.4 Molecular Liquids -- 5.5 Microscopic Models for Water -- 5.6 Some More Hints -- 5.7 Direct Calculations of the Equation of State -- 5.8 Free Energy Calculation from Thermodynamic Integration -- 5.9 An Example: Liquid-Solid Transition -- 5.10 Calculation of the Chemical

Potential: The Widom Method -- 5.11 Sampling in a Complex Energy Landscape -- 5.12 Umbrella Sampling -- 5.13 Histogram Methods -- 5.14 Free Energy Along a Reaction Coordinate -- 5.14.1 Umbrella Sampling for Reaction Coordinates -- 5.14.2 Metadynamics -- 5.15 Simulation of Critical Phenomena.

References -- 6 Dynamical Correlation Functions and Linear Response Theory for Fluids -- 6.1 Dynamical Observables -- 6.2 Correlation Functions -- 6.2.1 Further Properties of the Correlation Functions -- 6.3 Linear Response Theory -- 6.4 Dynamical Response Functions -- 6.5 Fluctuation-Dissipation Theorem -- 6.6 Response Functions and Dissipation -- 6.7 Density Correlation Functions and Van Hove Functions -- 6.8 Neutron Scattering to Determine the Liquid Dynamics -- 6.9 Dynamic Structure Factor -- 6.9.1 Static Limit -- 6.9.2 Incoherent Scattering -- 6.10 Density Fluctuations and Dissipation -- 6.10.1 Detailed Balance -- 6.11 Static Limit of the Density Fluctuations -- 6.12 Static Response Function and the Verlet Criterion -- References -- 7 Dynamics of Liquids -- 7.1 Thermal Motion in Liquids -- 7.2 Brownian Motion and Langevin Equation -- 7.3 Diffusion and Self Van Hove Function -- 7.4 Limit of the Dilute Gas -- 7.5 Short Time Expansion of the Self-Intermediate Scattering Function -- 7.6 Correlation Functions of the Currents -- 7.7 The Hydrodynamic Limit -- 7.8 Diffusion in the Hydrodynamic Limit -- 7.9 Velocity Correlation Function -- 7.10 Liquid Dynamics in the Hydrodynamic Limit -- 7.10.1 Transverse Current -- 7.10.2 Equations Under Isotherm Conditions, Longitudinal Current and Sound Waves -- 7.10.3 Longitudinal Current in Presence of Thermal Diffusion and Brillouin Scattering -- 7.11 Different Regimes for the Liquid Dynamics: The De Gennes Narrowing -- 7.12 Introduction of Memory Effects -- 7.12.1 The Langevin Equation and Memory Effects -- 7.12.2 Viscoelasticity: The Maxwell Model -- 7.12.3 Generalized Viscosity and Memory Effects -- 7.13 Definition of Memory Functions -- 7.14 Memory Function for the Velocity Correlation Function -- References -- 8 Supercooled Liquids: Glass Transition and Mode Coupling Theory.

8.1 Phase Transitions and Metastability of Liquids -- 8.2 Liquids Upon Supercooling: From the Liquid to the Glass -- 8.3 Angell Plot -- 8.4 Kauzmann Temperature -- 8.5 Adam and Gibbs Theory -- 8.5.1 Cooperative Rearranging Regions -- 8.5.2 Calculation of the Configurational Entropy -- 8.6 Energy Landscape and Configurational Entropy -- 8.7 Dynamics of the Supercooled Liquid and Mode Coupling Theory -- 8.7.1 Dynamics Upon Supercooling -- 8.7.2 Mode Coupling Theory and Cage Effect -- 8.7.3 Formulation of the Theory -- 8.7.4 Glass Transition as Ergodic to Non-ergodic Crossover -- 8.7.5 The -Relaxation -- 8.7.6 -Relaxation -- References -- 9 Supercooled Water -- 9.1 Supercooled and Glassy Water -- 9.2 The Hypothesis of a Liquid-Liquid Critical Point -- 9.3 The Widom Line at the Liquid-Liquid Transition -- 9.4 Water as a Two-Component Liquid -- 9.5 Dynamical Properties of Water Upon Supercooling -- 9.6 Widom Line and the Fragile to Strong Crossover -- References -- Index.
