

Contents

1 Structure of Hard Spheres and Related Systems	
<i>A. Malijevský and J. Kolafa</i>	1
1.1 Basic Concepts	1
1.2 Low-Density Region	4
1.3 High-Density Region	9
References	24
2 Introduction to the Thermodynamics of Hard Spheres and Related Systems	
<i>A. Malijevský and J. Kolafa</i>	27
2.1 Virial Coefficients of Pure Hard Spheres and Disks	27
2.2 Chemical Potentials of Hard Spheres and Related Systems	31
References	35
3 Equations of State for Hard Spheres and Hard Disks	
<i>A. Mulero, C.A. Galán, M.I. Parra and F. Cuadros</i>	37
3.1 Introduction	37
3.2 Equations of State for Hard Disks	40
3.3 Equations of State for Hard Spheres	60
3.4 Other Properties of the Hard-Sphere Fluid from Equations of State	96
3.5 Final Remarks	102
References	103
4 Application of Hard-Sphere and Hard-Disk Equations of State to the Weeks–Chandler–Andersen Reference System	
<i>A. Mulero, C.A. Galán, I. Cachadiña and F. Cuadros</i>	111
4.1 Introduction	111
4.2 Analytical Expressions	113
4.3 Pressure of the Three-Dimensional WCA RS	114
4.4 Potential Energy of the Three-Dimensional WCA RS	120
4.5 Pressure and Potential Energy of the Two-Dimensional WCA RS	121

4.6	Conclusions	128
	References	131

5 Binary Mixtures of Additive Hard Spheres. Simulations and Theories

	<i>C. Barrio and J.R. Solana</i>	133
5.1	Introduction	133
5.2	Computer Simulations	135
5.3	Consistency Conditions	147
5.4	Virial Coefficients	150
5.5	Contact Values of the Radial Distribution Functions, Equation of State, and Consistency	161
5.6	Deriving Density Expansions of the Contact Values of the Radial Distribution Functions from the Approximate Virial Expansion and Consistency Conditions	172
5.7	Rescaling the Density Expansions	176
5.8	Final Remarks	179
	References	180

6 Alternative Approaches to the Equilibrium Properties of Hard-Sphere Liquids

	<i>M.López de Haro, S.B. Yuste and A. Santos</i>	183
6.1	Introduction	183
6.2	Contact Values and Equations of State for Mixtures	185
6.3	The Rational Function Approximation (RFA) Method for the Structure of Hard-Sphere Fluids	211
6.4	Other Related Systems	224
6.5	Perturbation Theory	235
6.6	Perspectives	240
	References	241

7 Density Functional Theories of Hard Particle Systems

	<i>P. Tarazona, J. A. Cuesta and Y. Martínez-Ratón</i>	247
7.1	Introduction	247
7.2	Brief Tutorial to the Density Functional Formalism	248
7.3	The Exact Density Functional for Hard Rods	254
7.4	The Weighted Density Approximation	255
7.5	The Fundamental Measure Theory	270
7.6	Density Functionals for Hard Sphere Mixtures	290
7.7	Weighted Density Approximation for Mixtures of Hard Spheres ..	292
7.8	Fundamental Measure Theory for Mixtures of Hard Spheres	295
7.9	Non-Additive Mixtures of Hard Spheres	300
7.10	Density Functionals for Anisotropic Bodies	304
7.11	Fundamental Measure Theory for Anisotropic Particles	318
7.12	Summary	334
	References	336

8 Ensemble Effects in Small Systems

<i>F.L. Román, J.A. White, A. González and S. Velasco</i>	343
8.1 Velocity Distributions in Hard Particle Systems	345
8.2 Density Fluctuations in Hard-Particle Systems	357
8.3 Density Profiles of Inhomogeneous Systems. Structural Properties	369
References	379

9 Modelling of Transport Properties of Hard Sphere Fluids and Related Systems, and its Applications

<i>C.M. Silva and H. Liu</i>	383
9.1 Introduction	383
9.2 Molecular Dynamics Simulations	387
9.3 Theories of Transport in Hard Sphere and Modified Systems	391
9.4 Diffusion Coefficient	420
9.5 Viscosity	459
9.6 Thermal Conductivity	472
9.7 Conclusions and Final Remarks	485
References	487

10 Kinetic Theory for Binary Granular Mixtures at Low Density

<i>V. Garzó</i>	493
10.1 Introduction	493
10.2 Boltzmann Kinetic Equation for Binary Mixtures of Inelastic Hard Spheres	497
10.3 Homogeneous States	500
10.4 Navier–Stokes Hydrodynamic Equations	503
10.5 Comparison with Monte Carlo Simulations	507
10.6 Einstein Relation in Granular Gases	512
10.7 Onsager’s Reciprocal Relations in Granular Gases	514
10.8 Linearized Hydrodynamic Equations and Stability of the Homogeneous Cooling State	516
10.9 Segregation in Granular Binary Mixtures: Thermal Diffusion	521
10.10 Steady States: Uniform Shear Flow	528
10.11 Summary and Concluding Remarks	533
References	537

Index	541
--------------------	-----