Cambridge University Press 0521822157 - The Potential Distribution Theorem and Models of Molecular Solutions Thomas L. Beck, Michael E. Paulaitis and Lawrence R. Pratt Index More information

Index

 $\langle \langle \ldots \rangle \rangle_0$ notation, 18 n-to-k-falling notation, 48 ab initio molecular dynamics (AIMD) H⁺(aq), 210 k+(aq), Ho-(aq), 203 Li+(aq), Na+(aq), and K+(aq) compared, 199 water, 195 activity coefficients, 51 bias, 118 bootstrap methods, 119 Born model, 11, 68 central force models, 4, 54 chain-molecule chemical potentials and equations of state, 172 chain-molecule solutions, 172 cluster contributions in QCT, 146 general term, 147 order-by-order, 147 conditional expectation, 18 conditional probability, 18 configurational bias, Monte Carlo, 178 contact potentials, 70 cumulants, 105, 128 default model for information theories of primitive hydrophobiticy cluster Poisson model, 184 flat default model, 182 hard sphere model, 183 Lennard-Jones model, 184 Poisson default model, 182 practically perfect tetrahedral model, 185 density functional perspective on chemical potentials, 135 density functional theory, 132 dielectric constant, xi Egelstaff-Widom correlation length, 198 ensemble dependence of PDT, 43

entropy from the trajectory, 103 equilibrium ratios ideal, 24 non-ideal, 146 Ewald lattice sums, 112 Ewald potential, 108 examples bacterial Cl⁻ channel structure, 15 Be²⁺(aq), 149 ion channels, 13 K⁺(aq), 157 Nafion®, 9 reversed phase liquid chromatography (RPLC), 5 triflic acid, 9 water and AIMD, 153 Feynman-Hibbs model, 55

Flory–Huggins theory, 173 fluctuations, 27 functionals and functional derivatives, 132

gaussian density fluctuation theories, 65 gaussian extension of van der Waals model, 64 generalized Flory–Huggins theory, 178 glossary, xi

H/D isotope effects for aqueous solutions, 53 Hebb rule, 100 historical quasi-chemical calculation, 166 historical sketch, 2 hydrostatic linear response theory, 138 hypernetted chain approximation, 138

importance sampling, 100 inclusion–exclusion, 123 information model of primitive hydrophobicity, 182 inhomogeneous systems, 44 insertion probability $p_{\alpha}(0|\mathcal{R}^n)$, 74 integral equation theories, 132 inverse potential distribution theorem, 42 inversely restricted sampling (IRS), 176

jackknife method, 119

entropy convergence of hydrophobicities, 187

Cambridge University Press 0521822157 - The Potential Distribution Theorem and Models of Molecular Solutions Thomas L. Beck, Michael E. Paulaitis and Lawrence R. Pratt Index More information

230

Kirkwood-Buff theory, 140

Index

potential of the phase, 69

Kirkwood-Salsburg expansion, 123, 129 Mayer f function, 124 Mayer-Montroll expansion, 123 models association model, 94 continuum dielectric - Born - models, 67 Debye-Hückel theory, 89, 132 Flory-Huggins, 78 multigaussian, 70, 169 packing in fluids, 73 van der Waals theory, 61 Monte Carlo methods for chain molecules, 175 multigaussian models electrostatics, 70 packing, 169 nonuniformities: PY and HNC integral equations, 137 normalization of conformational distribution functions, $s_{\alpha}^{(0)}(\mathcal{R}^n)$, 18 Ornstein-Zernike (OZ) equation, 135 osmotic equation of state, 173 overlap methods, 104 partial molar entropy Born model, 12 primitive quasi-chemical model, 98 partial molar volume Born model, 11 primitive quasi-chemical model, 97 partioning of possibilities in ion clusters, 95 PDT formula for averages, 41 Percus-Yevick approximation, 138 perturbation theory, 105, 106 potential distribution theorem (PDT)

derivation, 39 partition function perspective, 33 inverse, 42 proximal radial distribution functions, 20 quantum generalization of the PDT, 53 quantum PDT, 56 quantum statistical mechanical models, 54 quasi-chemical theory (QCT) analysis of AIMD data, 153 Be²⁺(aq) example, 149 clustering in QCT, 146 derivation of the basic quasi-chemical formula, 143 H⁺(aq) example, 208 HO⁻(aq) example, 200 association model, 94, 145 explicit-implicit solvent models, 168 introduction, 142 packing, 157

realizability, 69 reduced distribution functions, 47 reference systems, 100 RISM theories, 140 Rosenbluth sampling, 176

scaled particle theory, 3 self consistent molecular field for packing, 160 son-of-superposition approximation, 179 stratification, 120 susceptibilities, 27, 63, 134, 138, 165

thermodynamic integration, 116

umbrella sampling, 100 Ursell expansion, 126 Ursell functions, 126

water as the matrix of life, 195
weak field limit of the chemical potential in an external field, 40
what are we to tell students about hydrophobicities?, 192
Wigner–Kirkwood model, 55