INDEX

acetic acid dimer, 326–329
adiabatic potential energy surfaces (APES)
  Jahn–Teller effect, 169–170
  Mexican hat, 170–171
  vibronic coupling constants, 171–172
anisotropic self-consistent variational potential (ASVP), 83–86
APES. see Adiabatic potential energy surfaces (APES)
associating fluids, 2
  bond saturation for hard spheres, 3
  cluster expansions
    Helmholtz free energy, 6–7
    hydrogen bonding, 7
    integral representations of graphs, 6
    Mayer functions, 5–6
    pair correlation function, 6
conical association sites, 4–5
density functional theory, 42–44
multiple association sites, 21–28
pair potential energy, 3
single association site
  bond renormalization, 8–10
  monovalent, 3
two-density formalism, 10–20
spherically symmetric and directional association sites
  cluster partition function, 41
  graph sum, pictorial representation, 40
  Monte Carlo simulation vs. theoretical predictions, 41–42
Smith and Nezbeda model, 39
two-site AB case
  bond cooperativity, 36–39
  linear triatomic clusters, 28
  ring formation, 32–36
  steric hindrance in chain formation, 29–32
Veytsman’s approach, 2
ASVP. see anisotropic self-consistent variational potential (ASVP)
atomic systems, in SSB
  finite-size, 164–166
  laws, 162
  multiminimum systems, 167–168
  Pierre Curie’s principle formulation, 166–168
  thermodynamic limit, 163–164
  two state paradigm, 187–190
avoided crossing. see pseudodegeneracy
backward evolution equations, 267–269
backward Fokker–Planck approach, 279–281
backward FPE, 272–273
backward master equation (BME), 267–269, 272–273
benzoic acid dimer, 326–329
BME. see backward master equation (BME)
Car–Parrinello molecular dynamics (CPMD), 326–327
channel transport
  continuous coordinate representation, 279–281
  discrete channel representation, 276–279
  long chains translocations, 285–287
  multiple particles in, 282–285
  one-dimensional diffusion, 281–282
  schematic representations, 276, 277
  charged point dipoles, 222–223
  conical square well (CSW) association sites, 4–5
  Coriolis splitting, 184
CPMD. see Car–Parrinello molecular dynamics (CPMD)
degeneracy induced by SSB
avoidance, 201–204
in elementary particle physics, 199–201
gas-liquid transition, 192–193
hidden degeneracy and pseudodegeneracy, 182–186
in interatomic and intermolecular interactions, 190–192
Jahn–Teller effect, 168–170
liquid-solid transition, 193–194
in polyatomic systems, 170–175
pseudodegeneracy with PJTE, 175–182
two state paradigm, 187–190
density functional theory (DFT), 42–44
DFT. see density functional theory (DFT)
diffraction effects, quantum fluid structure
continuous linear response, 95–99
instantaneous case, 93–95
observations and centroid structures, 99–102
quantum-effective pair potential structures, 103–108
TILB structures, 102–103
dipolar Poisson–Boltzmann (PB) equation, 215–219
direct correlation functions, quantum fluid structure
application, 112–115
BDH process, 111–112
Ornstein–Zernike equation, 108–111
directional association sites, 39–42
dumbbell ions, 240–241
entropy, 87, 128, 141, 163
excited electronic state, 334–336
finite-$P$ primitive approximation, 58–63
finite-size atomic systems, in SSB, 164–166
finite-spread Poisson–Boltzmann (PB) equation
dumbbell ions, 240–241
needle ions, 238–240
smeared-out charges, 229
spherical distribution, 230–238
first-passage processes
applications
channel transport, 276–287
receptor binding and adhesion, 287–290
single-cell growth and division, 290–300
backward evolution equations, 267–269
extrinsic noise, 262
Kramers’ method, 275–276
with multiple absorbing states, 273–275
stochastic processes, 263
time evolution equations, 264–267
using BME and backward FPE, 272–273
using FME and FPE, 269–271
fluid hydrogen, 133–135
FME method. see forward master equation (FME) method
Fokker–Planck equation (FPE), 265–266, 269–271
forward master equation (FME) method, 269–271, 276–279
FPE. see Fokker–Planck equation (FPE)
gas-liquid transition, 192–193
gauge transformation symmetry, 199
Gaussian core model, 211
Gaussian–Feynman–Hibbs (GFH) potential, 81–83
GFH potential. see Gaussian–Feynman–Hibbs (GFH) potential
helium fluids, 135–136
Helmholtz free energy, 6–7, 35, 125, 128
hidden degeneracy and pseudodegeneracy
ab initio calculations
CuF3, 185–186
ozone molecule, 182–183
APES cross section, 184
bistabilities, 186
Higgs potential, 200–201
higher-order propagators
primitive propagator, 63–64
SCVJ propagator, 65–66
TILB, 64–65
$H^+(H_2O)_n$ clusters, 336
anharmonic theoretical calculations, 337
instanton theory of tunneling splittings, 338
SCRF/IPCM calculations, 339
ultrafast dynamics, 340
hydrogen-bonded systems
acetic and benzoic acid dimers, 326–329
$\beta$-oxalic acid crystal, 320–323
$H^+(H_2O)_n$ clusters, 336–340
imidazole crystal, 325–326
infrared spectra model, 313–317
mechanisms, 329–330
1-methylthymine crystal, 317–319
1-methyluracil crystal, 320
proton tunneling, 334–336
salicylic acid crystal, 323–324
vibrational spectra, ices and aqueous solutions, 330–334
hydrogen bonding fluids, 7
imidazole crystal, 325–326
infrared (IR) spectra, hydrogen-bonded crystals, 329–330
interatomic and intermolecular interactions, 190–192
internal energy, 19–20, 27, 126, 140, 163
isotropic self-consistent variational potential (ISVP), 83–86
ISVP. see isotropic self-consistent variational potential (ISVP)
Jahn–Teller effect (JTE), 168–170
JTE. see Jahn–Teller effect (JTE)
Kramers’ method, 275–276
Kramers–Moyal expansion, 265–266
Langevin equation, 266–267
Langevin Poisson–Boltzmann (PB) equation, 219–222
liquid neon, 132–133
liquid-solid transition, 193–194
master equation (ME), 264–265
Mayer functions, 5–6
ME. see master equation (ME)
mean field approximation, 210–213
mean field electrostatics approximation, 211–213
effective one-body external potential, 210
finite-spread PB equation, 229
dumbbell ions, 240–241
needle ions, non-spherical distribution, 238–240
smeared-out charges, 230
spherical distribution, 230–238
Gaussian core model, 211
point-ion with structure
charged point dipoles, 222–223
dipolar PB equation, 215–219
Langevin PB equation, 219–222
polarizable PB equation, 223–229
standard PB equation, 213–215
1-methylthymine crystal, 317–319
1-methyluracil crystal, 320
monatomic fluids at equilibrium. see quantum monatomic 3D fluids
Monte Carlo simulation
associating fluids, 41–42
path integrals approach, 75–77
quantum monatomic 3D fluids, 141–142
spherical distribution, 235
multi-density approach approximations, 27–28
bonding, 23–24
pair correlation function, 26
TPT1, 26–27
two-site-associating fluids, 21
multivalent binding and adhesion avidity, 289
viral dissociation, endocytosis, and fusion, 289–290
viral particle binding and dissociation at cell surface, 287–289
non-spherical distribution, needle ions, 238–240
Ornstein–Zernike equation, 108–111
β-oxalic acid crystal, 320–323
pair product actions
counterpart of hard spheres, 69
JOHS and CBHS propagators, 69–71
quantum hard spheres, 66–71
pairwise additivity, 28
patchy colloids, 2
path integrals (PI) approach
convolutions and sum over histories, 56–58
finite-\( P \) primitive approximation, 58–63
higher-order propagators, 63–66
molecular dynamics and Monte Carlo techniques, 75–77
pair product actions, 66–71
quantum exchange, 71–74
quantum partition function, 54–56
PI approach. see path integrals (PI) approach
Pierre Curie’s principle, 166–168
PJTE. see pseudo JTE (PJTE)
polarizable Poisson–Boltzmann (PB) equation, 223
counter value theorem, 225
dielectric constant, 226, 227
frequency-dependent, 224
mean potential, 224
negative excess polarizability, 226, 228–229
polyatomic systems, in SSB
degeneracy, 170–175
hidden degeneracy and pseudodegeneracy, 182–186
Jahn–Teller effect, 168–170
pseudodegeneracy, 175–182
proton tunneling, in symmetrical double-well potential, 334–336
pseudodegeneracy
covalence origin, 181–183
electronic energy-level diagram, 180
PJTE, 176
pseudorotations, 178–179
puckering, 177–178
Renner–Teller effect, 177
SSB induced by hidden degeneracy, 182–186
SSB in elementary particle physics, 201
structure of hemoglobin active site, 181
two state paradigm, 187–190
pseudo JTE (PJTE), 175–182
puckering, 177–178
QFH potentials. see quadratic Feynman–Hibbs (QFH) potentials
QHS. see quantum hard spheres (QHS)
quadratic Feynman–Hibbs (QFH) potentials, 81–83
quantum-effective pair potential structures
GFH picture, 104–107
instantaneous structure factor, 103
ISVP and ASVP, 107–108
quantum hard spheres (QHS), 66–71, 86–87
quantum monatomic 3D fluids
Boltzmann statistics, 51
numerical simulation
BDH evolution, TLR2 quantities, 148–149
BDH+GC calculations, 148, 150
centroid structure factors, 146–147
continuous linear response structure factors, 146–148
fluid helium-state points and computational methods, 136–137
fluid hydrogen, 133–135
GC iterations, 145
Gibbs free energies and entropies, 141
instantaneous structure factors, 146–147
internal energies and pressures, 140
isothermal compressibilities, 143–144
liquid neon, 132–133
Metropolis algorithm, 136
Monte Carlo pair radial correlation functions, 141–142
pair direct correlation functions, 150–151
P-convergence properties, 138–139
PIMC(AZS) pair radial correlation functions, 142–143
QHS, bare (QHS), and QHSY fluid, 131–132
stable isotope helium fluids, 135–136
path integrals approach
advantages, 50
convolutions and sum over histories, 56–58
finite-P primitive approximation, 58–63
higher-order propagators, 63–66
molecular dynamics and Monte Carlo techniques, 75–77
pair product actions, 66–71
quantum exchange, 71–74
quantum partition function, 54–56
semiclassical approaches
advantages, 79
path integrals, 79–86
quantum hard spheres, 86–87
Wigner–Kirkwood expansion, 78–79
statistical ensembles, 51–52
structural properties
asymptotic behavior, quantum pair correlations, 115–116
correlation functions, 87
direct correlation functions, 108–115
grand partition function, 91
instantaneous and total continuous linear response, 88–89
pair direct correlation function, 90
pair level/diffraction effects, 93–108
P beads per actual particle, 92
PI fluid structures, 124–125
quantum triplet correlations, 116–121
static structure factors, 87
triplet quantum-response functions, 121–124
thermodynamic properties
adiabatic switching and reversible scaling methods, 131
complementary measure, 130
estimators, 126
isothermal compressibility, 128
kinetic energy and Helmholtz free energy, 125
necklace centroids, 127
PI quantum effective pair potentials, 130
TILB estimators, 127
Widom method, 129
quantum pair correlations, 115–116
quantum partition function, 54–56
quantum triplet correlations, 116–121
Raman spectra, hexagonal and cubic ice, 330–334
Renner–Teller effect (RTE), 177
RTE. see Renner–Teller effect (RTE)
salicylic acid crystal, 323–324
SDE. see stochastic differential equations (SDE)
self-consistent variational potentials (SVP), 83–86
semiclassical partition function
centroid concept, 78–79
PI based approaches
GFH picture, 81–83
self-consistent variational potentials, 83–86
quantum effective pair potentials, 79–80
quantum hard spheres, 86–87
Taylor expansions, 81
Wigner–Kirkwood expansion, 78–79
short-range non-electrostatic interactions, 241
correlations, 251–252
electrostatic potential, 256, 257
free energy, 246–247
lattice gas equation, 254
local approximation, 252–253
mean field implementation
cations, anions, and total charge near uncharged wall, 245
counterions near charged wall, 244
penetrable sphere ions, 242–243
modified PB equation vs. other approximations, 255, 256
nonperturbative approach, 248–251
perturbative expansion and dilute limit, 247–248
single association site
bond renormalization, 8–10
monovalent, 3
two-density formalism
divalent case, 14–20
fugacity expansion, 10
graphical representation, 11–12
monovalent case, 12–14
single-cell growth and division
biological context, 290–291
cell cycle as phase oscillator, 297–298
FTP problem, cell division formulation, 291
ME approach, 294–297
phenomenological approach, Langevin dynamics, 298–300
scale invariance, FPT distribution, 293–294
sizes at division and interdivision times, 291–292
single chain approximation, 27
singly bondable association sites, 27
SMC potential. see symmetric mode coupling (SMC) potential
solid state phase transitions, 194–199
spherical distribution, 230
charge density and electrostatic potential, 233
co-ion density profile, 236
Monte Carlo configuration, 235
number density profiles, 234, 235
pair potential, 231, 232
stacked configurations, 237–238
spherically symmetric association sites, 39–42
spontaneous symmetry breaking (SSB)
in atomic systems
finite-size, 164–166
laws, 162
multiminimum systems, 167–168
Pierre Curie’s principle formulation, 166–168
thermodynamic limit, 163–164
two state paradigm, 187–190
degeneracy avoidance, 201–204
in elementary particle physics
gauge transformation symmetry, 199
Higgs potential, 200–201
pseudodegeneracy, 201
induced by degeneracy
gas-liquid transition, 192–193
in interatomic and intermolecular interactions, 190–192
liquid-solid transition, 193–194
in polyatomic systems
degeneracy, 170–175
hidden degeneracy and pseudodegeneracy, 182–186
Jahn–Teller effect, 168–170
pseudodegeneracy, 175–182
solid state phase transitions, 194–199
squeezed double-well potential (SQZ), 336
SQZ. see squeezed double-well potential (SQZ)

SSB. see spontaneous symmetry breaking (SSB)

stable isotope helium fluids, 135–136

standard Poisson–Boltzmann (PB) equation, 213–215

stochastic differential equations (SDE), 266–267

stochastic processes, 263

SVP. see self-consistent variational potentials (SVP)

symmetric mode coupling (SMC) potential, 336

thermodynamic perturbation theory (TPT), 14–20

thermodynamic properties, quantum fluids

adiabatic switching and reversible scaling methods, 131
complementary measure, 130
estimators, 126
isothermal compressibility, 128
kinetic energy and Helmholtz free energy, 125
necklace centroids, 127
PI quantum effective pair potentials, 130
TILB estimators, 127
Widom method, 129

time evolution equations
Kramers–Moyal expansion and FPE, 265–266
Langevin equation and SDE, 266–267
master equation, 264–265

TPT. see thermodynamic perturbation theory (TPT)

triplet quantum-response functions, 121–124
tropolone, 334–335
two-density approach

divalent case, 14–20
fugacity expansion, 10
graphical representation, 11–12
monovalent case, 12–14

Veytsman’s approach, 2

vibrational spectra
bond-dipole and bond polarizability models, 330
ferroelectric ice in solar system and galaxy, 334
hexagonal ice, experimental vs. calculated, 331
infrared spectra, HDO molecules, 332–333
Morse oscillator, 330
parallel-polarized Raman spectra, isotopic cubic ice mixtures, 331–332