

Index

A

action principle

- 1.1: The Lagrangian Formulation of Classical Mechanics

anticommutator

- 13.1.2: The Transition Rate

C

caging

- 14.3: The Dynamic Friction Kernel

canonical partition function

- 4.3: Relation between Canonical and Microcanonical Ensembles

Classical Virial Theorem

- 3.3: The Classical Virial Theorem (Microcanonical Derivation)

closure

- 9.1: Measurement

collective variables

- 8.4: Reaction Coordinates

configurational partition function

- 7.2: General Distribution Functions and Correlation Functions

confocal elliptic coordinates

- 8.4: Reaction Coordinates

conjugate momenta

- 1.2: The Hamiltonian formulation of classical mechanics

D

density matrix

- 10.2: The Density Matrix and Density Operator

density operator

- 10.2: The Density Matrix and Density Operator

diffusion constant

- 12.8.2: The Diffusion Constant

distribution functions

- 7.1: General Formulation of Distribution Functions

E

ensemble

- 1.5: Classical microscopic states or microstates and ensembles

- 2.1: The Ensemble Concept (Heuristic Definition)

equal a priori probabilities

- 3: The Microcanonical Ensemble

equations of motion

- 1.1: The Lagrangian Formulation of Classical Mechanics

equilibrium time correlation function

- 12.5: Perturbative solution of the Liouville equation

Euclidean action

- 11.1.3: Dominant Paths in the Propagator and Density Matrix

Euler's theorem

- 6.1: Thermodynamics

expectation value

- 11.2.1: Expectation values of observables

F

Fermi's Golden Rule

- 13.4: Fermi's Golden Rule

free energy hypersurface

- 8.4: Reaction Coordinates

fugacity

- 6.2: Partition Functions

functional integral

- 11.1.4: The Continuous Limit

G

general correlation function

- 7.4: General Correlation Functions

generalized equations of motion

- 12.3: Generalized Equations of Motion

Generalized Langevin Equation

- 14.3: The Dynamic Friction Kernel

generalized Liouville equation

- 2.2: Liouville's Theorem for non-Hamiltonian systems

H

Hamiltonian operator

- 13.1.1: The Hamiltonian

harmonic bath

- 14.1: The Harmonic Bath Hamiltonian

Heisenberg picture

- 9.4: The Heisenberg Picture

Heisenberg uncertainty principle

- 9.5: The Heisenberg Uncertainty Principle

Hemholtz energy

- 3.1: Basic Thermodynamics

Hermitian operators

- 9.1: Measurement

Hilbert space

- 9.6: The Physical State of a Quantum System

I

imaginary time path integral

- 11.1.4: The Continuous Limit

interaction picture

- 13.2: Iterative solution for the interaction-picture state vector

- 13.3: The Interaction Picture

J

Jarzynski's equality

- 8.5: Jarzynski's Equality and Nonequilibrium Methods

K

Kubo transform

- 12.2: Kubo Transform Expression for the Time Correlation Function

L

Lagrangian

- 1.2: The Hamiltonian formulation of classical mechanics

Langevin equation

- 14.3: The Dynamic Friction Kernel

Legendre Transforms

- 4.2: Legendre Transforms

Liouville equation

- 2.3: The Liouville Operator and the Poisson Bracket
- 12.5: Perturbative solution of the Liouville equation

Liouville operator

- 2.3: The Liouville Operator and the Poisson Bracket

Liouville's Theorem

- 1.6: Phase space distribution functions and Liouville's theorem
- 2.2: Liouville's Theorem for non-Hamiltonian systems
- 4.4: Preservation of Phase Space Volume and Liouville's Theorem

M

Maslov index

- 11.3.2: The Stationary Phase Approximation

memory integral

- 14.3: The Dynamic Friction Kernel

microcanonical ensemble

- 3: The Microcanonical Ensemble

Microscopic Laws of Motion

- 1.3: The Microscopic Laws of Motion

microscopic state

- 1.5: Classical microscopic states or microstates and ensembles

microstate

- 1.5: Classical microscopic states or microstates and ensembles

O

Onsager fluctuation regression theorem

- 12.6: The Onsager Fluctuation Regression Theorem

Onsager regression hypothesis

- 12.4: General Properties of Time Correlation Functions

order parameters

- 8.4: Reaction Coordinates

P

pair correlation function

- 7.6: The Pair Correlation Function

partition functions

- 6.2: Partition Functions

path integrals

- 11.1: Discretized and Continuous Path Integrals

phase space

- 1.4: Phase Space

phase space distribution function

- 1.6: Phase space distribution functions and Liouville's theorem

phase space probability density

- 1.6: Phase space distribution functions and Liouville's theorem

Poisson bracket

- 2.3: The Liouville Operator and the Poisson Bracket

pressure tensor

- 12.8.1: Shear Viscosity

principle of least action

- 11.1.3: Dominant Paths in the Propagator and Density Matrix

Q

quantum Liouville equation

- 13.1.2: The Transition Rate

quantum propagator

- 9.7: Time Evolution of the State Vector

R

reaction coordinate

- 8.4: Reaction Coordinates

S

saddle point approximation

[11.3.2: The Stationary Phase Approximation](#)

Schrödinger picture

[9.4: The Heisenberg Picture](#)

shear force

[12.8.1: Shear Viscosity](#)

shear viscosity

[12.8.1: Shear Viscosity](#)

solvent cage

[14.3: The Dynamic Friction Kernel](#)

stationary phase approximation

[11.3.2: The Stationary Phase Approximation](#)

superoperator

[10.3: Time evolution of the density operator](#)

switching functions

[8.3: Adiabatic Switching and Thermodynamic Integration](#)

T

tetradic operator

[10.3: Time evolution of the density operator](#)

thermal de Broglie wavelength

[11.1.2: Doing the Path Integral - the Free Particle](#)

thermodynamic limit

[4.5: Energy Fluctuations in the Canonical Ensemble](#)

time evolution operator

[9.7: Time Evolution of the State Vector](#)

trajectory

[1.1: The Lagrangian Formulation of Classical Mechanics](#)

transition rate

[13.1.2: The Transition Rate](#)

transport coefficient

[12.8.1: Shear Viscosity](#)

V

van der Waals equation

[7.7: Derivation of the Van der Waals equation](#)

velocity autocorrelation function

[12.8.2: The Diffusion Constant](#)

virial equation of state

[7.5: Thermodynamic quantities in terms of \$g\(r\)\$](#)

virial theorem

[4.1: Classical Virial Theorem \(Canonical Ensemble Derivation\)](#)

W

Wick rotation

[11.1.4: The Continuous Limit](#)

work virial theorem

[5.2: Pressure and Work Virial Theorems](#)