

## HEAT TRANSFER PHYSICS, SECOND EDITION

This graduate textbook describes atomic-level kinetics (mechanisms and rates) of thermal energy storage, transport (conduction, convection, and radiation), and transformation (various energy conversions) by principal energy carriers. The approach combines the fundamentals of molecular orbitals-potentials, statistical thermodynamics, computational molecular dynamics, quantum energy states, transport theories, solid-state and fluid-state physics, and quantum optics. The textbook presents a unified theory, over fine-structure/molecular-dynamics/Boltzmann/macroscale length and time scales, of heat transfer kinetics in terms of transition rates and relaxation times, and its modern applications, including nano- and microscale size effects. Numerous examples, illustrations, and homework problems with answers to enhance learning are included. This new edition includes applications in energy conversion (including chemical bond, nuclear, and solar), expanded examples of size effects, inclusion of junction quantum transport, and discussion of graphene and its phonon and electronic conductances. New appendix coverage of phonon contributions to the Seebeck coefficient, Monte Carlo methods, and ladder operators is also included.

Massoud Kaviany is a Professor in the Department of Mechanical Engineering and in the Applied Physics Program at the University of Michigan, where he has been since 1986. His area of teaching and research is heat transfer physics, with a particular interest in porous media. His current projects include atomic structural metrics in high-performance thermoelectric materials (both electron and phonon transport) and in laser cooling of solids (including *ab initio* calculations of photon-electron and electron-phonon couplings), and the effect of pore water in polymer electrolyte transport and fuel cell performance. His integration of research into education is currently focused on heat transfer physics, treating the atomic-level kinetics of transport and interaction of phonon, electron, fluid particle, and photon in a unified manner. It combines *ab initio* (fine structure), molecular dynamics, Boltzmann transport, and macroscopic treatments, but on increasing length and times scales. He is author of the monographs *Principles of Heat Transfer in Porous Media* (2nd Ed.) and *Principles of Convective Heat Transfer* (2nd Ed.), and the undergraduate textbooks *Principles of Heat Transfer* and *Essentials of Heat Transfer*. He received the College of Engineering's Education Excellence Award in 2003. He is an editor of the *Journal of Nanoscale and Microscale Thermophysical Engineering* and is on the editorial board of the *International Journal of Heat and Mass Transfer* and several other international journals. He is an ASME Fellow (since 1992) and an APS Fellow (since 2011), was Chair of the ASME Committee on Theory and Fundamental Research in Heat Transfer (1995–98), and is the recipient of the 2002 ASME Heat Transfer Memorial Award (Science) and the 2010 Harry Potter Gold Medal (Thermodynamics Science).

Cambridge University Press  
978-1-107-04178-3 - Heat Transfer Physics: Second Edition  
Massoud Kaviany  
Frontmatter  
[More information](#)

---

Cambridge University Press  
978-1-107-04178-3 - Heat Transfer Physics: Second Edition  
Massoud Kaviany  
Frontmatter  
[More information](#)

---

# Heat Transfer Physics

Second Edition

Massoud Kaviany  
*University of Michigan*



Cambridge University Press  
978-1-107-04178-3 - Heat Transfer Physics: Second Edition  
Massoud Kaviany  
Frontmatter  
[More information](#)

**CAMBRIDGE**  
UNIVERSITY PRESS

32 Avenue of the Americas, New York, NY 10013-2473, USA

Cambridge University Press is part of the University of Cambridge.

It furthers the University's mission by disseminating knowledge in the pursuit of education, learning, and research at the highest international levels of excellence.

[www.cambridge.org](http://www.cambridge.org)

Information on this title: [www.cambridge.org/9781107041783](http://www.cambridge.org/9781107041783)

© Massoud Kaviany 2008, 2014

This publication is in copyright. Subject to statutory exception and to the provisions of relevant collective licensing agreements, no reproduction of any part may take place without the written permission of Cambridge University Press.

First edition published 2008

Second edition 2014

Printed in the United States of America

*A catalog record for this publication is available from the British Library.*

*Library of Congress Cataloging in Publication Data*

Kaviany, M. (Massoud), author.

Heat transfer physics / Massoud Kaviany. – Second edition.

pages cm

Includes bibliographical references and index.

ISBN 978-1-107-04178-3 (hardback)

1. Nuclear reactor kinetics. 2. Change of state (Physics) 3. Heat storage. 4. Heat – Transmission.

I. Title.

QC787.N8K39 2013

536/.2–dc23 2013032185

ISBN 978-1-107-04178-3 Hardback

Cambridge University Press has no responsibility for the persistence or accuracy of URLs for external or third-party Internet Web sites referred to in this publication and does not guarantee that any content on such Web sites is, or will remain, accurate or appropriate.

Cambridge University Press  
978-1-107-04178-3 - Heat Transfer Physics: Second Edition  
Massoud Kaviany  
Frontmatter  
[More information](#)

---

*To curiosity, reason, doubt,  
dialogue, understanding, tolerance,  
and humility.*

Cambridge University Press  
978-1-107-04178-3 - Heat Transfer Physics: Second Edition  
Massoud Kaviany  
Frontmatter  
[More information](#)

---

## Contents

<i>Preface</i>	<i>page</i> xvii
<i>Acknowledgments</i>	xxi
<b>1 Introduction and Preliminaries . . . . .</b>	<b>1</b>
1.1 Principal Carriers: Phonon, Electron, Fluid Particle, and Photon	3
1.1.1 Phonon	4
1.1.2 Electron (and Hole)	7
1.1.3 Fluid Particle	8
1.1.4 Photon	9
1.2 Equilibrium and Nonequilibrium Energy Occupancy Distributions	10
1.2.1 Nonequilibrium Energy Carrier Occupancy by Energy Conversion	10
1.2.2 Transport Phenomena Related to Energy Occupancy Distributions	14
1.3 Particles, Waves, Wave Packets and Quasi-Particles, and Density of States	16
1.4 A History of Contributions Toward Heat Transfer Physics	17
1.5 Fundamental Constants and Fine-Structure Scales	20
1.5.1 Boltzmann and Planck Constants	20
1.5.2 Atomic Units and Fine-Structure Scales	21
1.6 Principal Carriers: Concentration, Energy, Kinetics, and Speed	23
1.6.1 Principal-Energy Carriers Concentration	24
1.6.2 Principal-Carrier Energy	25
1.6.3 Principal-Carrier Energy Transport/Transformation Kinetics	26
1.6.4 Principal-Carrier Speed	29
1.7 Periodic Table of Elements	29
	vii

1.8	Heat Transfer Physics: Atomic-Level Energy Kinetics	32
1.8.1	Thermal Energy Storage	32
1.8.2	Thermal Energy Transport	33
1.8.3	Thermal Energy Transformation	35
1.9	Density of States and Carrier Density	40
1.10	<i>Ab Initio</i> /MD/BTE/Macroscopic Treatments	42
1.11	Scope	44
1.12	Problems	46
<b>2</b>	<b>Molecular Orbitals/Potentials/Dynamics and Quantum Energy States . . . . .</b>	<b>50</b>
2.1	Interatomic Forces and Potential Wells	50
2.1.1	Interatomic Forces	52
2.1.2	Intermolecular Forces	52
2.1.3	Kinetic and Potential Energies and Potential Wells	53
2.2	Orbitals and Interatomic Potential Models	58
2.2.1	Atomic and Molecular Electron Orbitals	58
2.2.2	<i>Ab Initio</i> Computation of Interatomic Potentials	61
2.2.3	Potential Models and Phases	65
2.2.4	Examples of Atomic Bond Length and Energy	72
2.2.5	Radial Distribution of Atoms in Dense Phase	73
2.3	Molecular Ensembles, Temperature, and Thermodynamic Relations	75
2.3.1	Ensembles and Computational Molecular Dynamics	75
2.3.2	Energy Equipartition	75
2.3.3	Thermodynamic Relations	76
2.4	Hamiltonian Mechanics	77
2.4.1	Classical and Quantum Hamiltonians	77
2.4.2	Probability and Partition Function	79
2.4.3	Ergodic Hypothesis in Theoretical Statistical Mechanics	81
2.5	Molecular Dynamics Simulations	81
2.5.1	Ensemble and Discretization of Governing Equations	81
2.5.2	A Molecular Dynamics Simulation Case Study: L–J Ar FCC	86
2.5.3	L–J FCC MD Scales in Classical Harmonic Oscillator	88
2.5.4	L–J Potential Phase Transformations	92
2.5.5	Atomic Displacement in Solids and Quantum Effects	93
2.5.6	Specific Heat Capacity	94
2.5.7	Heat Flux Vector	95
2.6	Schrödinger Equation and Quantum Energy States	96
2.6.1	Time-Dependent Schrödinger Equation and Wave Vector	97
2.6.2	Bloch Wave Form	99



*Contents*

ix

2.6.3	Quantum-Mechanics Formalism, Bra–Ket and Matrix Element	100
2.6.4	Quantum Mechanical, Harmonic Oscillator	101
2.6.5	Periodic, Free Electron (Gas) Model for Metals	105
2.6.6	Electron Orbitals in Hydrogenlike Atoms	109
2.6.7	Perturbation and Numerical Solutions to Schrödinger Equation	111
2.7	Problems	115
<b>3</b>	<b>Carrier Energy Transport and Transformation Theories . . . . .</b>	<b>119</b>
3.1	Boltzmann Transport Equation	120
3.1.1	Particle Probability Distribution (Occupancy) Function	120
3.1.2	A Simple Derivation of BTE	120
3.1.3	In- and Out-Scattering	123
3.1.4	Relaxation-Time Approximation of Scattering and Transport Properties	124
3.1.5	Boltzmann Transport Scales	128
3.1.6	Momentum, Energy, and Average Relaxation Times	129
3.1.7	Moments of BTE	130
3.1.8	Numerical Solution to BTE	131
3.2	Energy Transition Kinetics and Fermi Golden Rule	131
3.2.1	Elastic and Inelastic Scattering	132
3.2.2	Phonon Interaction and Transition Rates	133
3.2.3	Electron (and Hole) Interaction and Transition Rates	134
3.2.4	Fluid Particle Interaction and Transition Rates	138
3.2.5	Photon Interaction and Transition Rates	138
3.3	Maxwell Equations and Electromagnetic Waves	138
3.3.1	Maxwell Equations	138
3.3.2	Electromagnetic Wave Propagation Equation	142
3.3.3	EM Wave and Photon Energy	144
3.3.4	Electric Dipole and Emission, Absorption, and Scattering of EM Waves	145
3.3.5	Dielectric Function and Dielectric Heating	147
3.3.6	Electrical Resistivity and Mobility and Joule Heating	151
3.4	Onsager Coupled Transport Coefficients	152
3.5	Stochastic Particle Dynamics and Transport	154
3.5.1	Langevin Particle Dynamics Equation and Brownian Motion	154
3.5.2	Fokker–Planck Particle Conservation Equation	155
3.5.3	Mean-Field Theory	155
3.6	Equilibrium Fluctuation–Dissipation and Green–Kubo Transport Theory	156
3.7	Macroscopic Fluid Dynamics Equations	159
3.8	Macroscopic Elastic Mechanics Equations	159

3.9	Macroscopic Scales	161
3.10	Problems	163
<b>4</b>	<b>Phonon Energy Storage, Transport, and Transformation Kinetics . . .</b>	<b>173</b>
4.1	Phonon Dispersion in One-Dimensional Classical Lattice Vibration	174
4.2	Phonon Density of States and Debye Model	181
4.2.1	Phonon DOS for One-Dimensional Lattice and van Hove Singularities	182
4.2.2	Debye and Other Phonon DOS Models	184
4.3	Reciprocal Lattice, Brillouin Zone, and Primitive Cell and Its Basis	186
4.3.1	Reciprocal Lattice	187
4.3.2	Brillouin Zone	189
4.3.3	Primitive Cell and Its Basis: Number of Phonon Branches	190
4.4	Normal Modes and Dynamical Matrix	191
4.5	Quantum Theory of Lattice Vibration	196
4.6	Examples of Phonon Dispersion and DOS	198
4.7	Phonon Specific Heat Capacity and Debye Average Acoustic Speed	201
4.7.1	Acoustic Phonon Specific Heat Capacity	201
4.7.2	Estimate of Directional Acoustic Velocity	206
4.8	Atomic Displacement in Lattice Vibration	208
4.9	Phonon BTE and Callaway Conductivity Model	211
4.9.1	Single-Mode Relaxation Time	211
4.9.2	Callaway Phonon Conductivity Model from BTE	212
4.9.3	Callaway–Holland Phonon Conductivity Model	215
4.9.4	Phonon Scattering Relaxation Time Models	215
4.9.5	Phonon Dispersion Models: Ge As Example	223
4.9.6	Comparison of Dispersion Models	226
4.9.7	Lattice Thermal Conductivity Prediction	228
4.10	Einstein and Cahill–Pohl Minimum Phonon Conductivities	231
4.11	Material Metrics of Phonon Conductivity: Slack Relation	233
4.11.1	Derivation of Slack Relation	234
4.11.2	Force-Constant Combinative Rule for Arbitrary Pair-Bond	235
4.11.3	Evaluation of Sound Velocity and Debye Temperature	241
4.11.4	Prediction of Grüneisen Parameter	244
4.11.5	Prediction of Thermal Conductivity	249
4.12	Phonon Conductivity Decomposition: Acoustic Phonons	254
4.12.1	Heat Current Autocorrelation Function	255
4.12.2	Phonon Conductivity Decomposition	258
4.12.3	Comparison with Experiment	260

## Contents

xi

4.13	Phonon Conductivity Decomposition: Optical Phonons	261
4.14	Quantum Corrections to MD/G-K Predictions	262
4.15	Phonon Conductivity from BTE: Variational Method	267
4.16	Experimental Data on Phonon Conductivity	269
4.17	Phonon Boundary Resistance	271
4.18	Absorption of Ultrasound Waves in Solids	275
4.19	Size Effects	276
4.19.1	Finite-Size Effect on Phonon Conductivity	276
4.19.2	Superlattice Phonon Conductivity	278
4.19.3	Phonon Density of States of Nanoparticles	280
4.19.4	Phonon Conductivity Rectification in Anisotropic, One-Dimensional Systems	286
4.19.5	Heat Flow in Molecular Wire	287
4.19.6	Quantum Vibrational Energy Flow in Nanostructures	288
4.19.7	Nanocone Conductivity	289
4.20	Problems	289
<b>5</b>	<b>Electron Energy Storage, Transport, and Transformation Kinetics . . .</b>	<b>306</b>
5.1	Schrödinger Equation for Periodic-Potential Electronic Band Structure	309
5.2	Electronic Band Structure in One-Dimensional Ionic Lattice	311
5.3	Three-Dimensional Bands Using Tight-Binding Approximation	315
5.3.1	General LCAO	315
5.3.2	Example of Tight-Binding Approximation: FCC, Single $s$ -Band	317
5.4	<i>Ab Initio</i> Computation of Electron Band Structure	319
5.5	Electron Band Structure for Semiconductors and Effective Mass	321
5.6	Periodic Electron Gas Model for Metals	325
5.7	Electron/Hole Density of Carrier and States for Semiconductors	327
5.8	Specific Heat Capacity of Conduction Electrons	331
5.9	Electron BTE for Semiconductors: Thermoelectric Force	334
5.10	Electron Relaxation Time and Fermi Golden Rule	335
5.11	Average Relaxation Time $\langle\langle\tau_e\rangle\rangle$ for Power-Law $\tau_e$ (Momentum) ( $E_e$ )	338
5.12	Thermoelectric Transport Property Tensors for Power-Law $\tau_e(E_e)$	343
5.13	TE Transport Coefficients for Cubic Semiconductors	346
5.13.1	Seebeck, Peltier, and Thomson Coefficients, and Electrical and Thermal Conductivities	346
5.13.2	Electron Mean Free Path for Metals	348
5.14	Magnetic Field and Hall Factor and Coefficient	349

5.15	Electron–Phonon Relaxation Times in Semiconductors	350
5.15.1	Electron–Phonon Wave Function	351
5.15.2	Rate of Acoustic-Phonon Scattering of Electrons	353
5.15.3	Rate of Optical-Phonon Scattering of Electrons	354
5.15.4	Summary of Electron-Scattering Mechanisms and Relaxation-Time Relations	359
5.16	TE Transport Coefficients Data for Metals and Semiconductors	359
5.16.1	Structural Defects in Crystalline Solids	359
5.16.2	Metals	360
5.16.3	Semiconductors	366
5.16.4	TE Figure of Merit $Z_e$	372
5.17	<i>Ab Initio</i> Computation of TE Transport Property Tensors	377
5.17.1	TE Transport Tensors and Variable Chemical Potential	377
5.17.2	Introduction to BoltzTraP	379
5.17.3	Relaxation Times Based on Kane Band Model	380
5.17.4	Predicted Seebeck Coefficient and Electrical Conductivity	385
5.17.5	Electric and Phonon Thermal Conductivities	388
5.18	Electron and Phonon Transport Under Local Thermal Nonequilibrium	393
5.18.1	Derivations	393
5.18.2	Phonon Modal Energy Equations	395
5.18.3	Summary of Conservation (Electrohydrodynamic) Equations	396
5.19	Cooling Length in Electron–Phonon Local Thermal Nonequilibrium	397
5.20	Electronic Energy States of Ions in Crystals	400
5.21	Electronic Energy States of Gases	404
5.22	Size Effects	407
5.22.1	Quantum Well for Improved TE $Z_e T$	408
5.22.2	Reduced Electron–Phonon Scattering Rate in Quantum Wells	411
5.22.3	Electronic and Phonon Thermal Conductance of Graphene–Flake Junctions	413
5.22.4	Heterobarrier for Converting Hot–Phonon Energy to Electric Potential	418
5.23	Problems	422
<b>6</b>	<b>Fluid Particle Energy Storage, Transport, and Transformation Kinetics . . . . .</b>	<b>434</b>
6.1	Fluid Particle Quantum Energy States and Partition Functions	436
6.1.1	Translational Energy and Partition Function	436
6.1.2	Vibrational Energy and Partition Function	438

*Contents*

xiii

6.1.3	Rotational Energy and Partition Function	439
6.1.4	Electronic Energy and Partition Function	440
6.1.5	<i>Ab Initio</i> Computation of Vibrational and Rotational Energy States	441
6.2	Ideal-Gas Specific Heat Capacity	443
6.3	Dense-Fluid Specific Heat Capacity: van der Waals Model	447
6.4	Gas BTE, $f_j^o$ , and Thermal Velocities	451
6.4.1	Interparticle Collisions	451
6.4.2	Equilibrium Distribution Function for Translational Energy	453
6.4.3	Inclusion of Gravitational Potential Energy	456
6.5	Ideal-Gas Binary Collision Rate and Relaxation Time	457
6.6	Ideal-Gas Mean Free Path and Viscosity	459
6.7	Kinetic-Limit Evaporation/Condensation Heat Transfer Rate	461
6.8	Ideal-Gas Thermal Conductivity from BTE	462
6.8.1	Nonequilibrium BTE and Relaxation-Time Approximation	462
6.8.2	Thermal Conductivity	463
6.9	Liquid Thermal Conductivity from Mean Free Path and Molecular Dynamics	469
6.10	Effective Conductivity with Dispersed Particles in Thermal Motion	470
6.10.1	Langevin Derivation of Brownian Diffusion	471
6.10.2	Thermal Relaxation Time and Effective Fluid Thermal Conductivity	472
6.11	Interaction of Moving Fluid Particle and Surface	474
6.11.1	Fluid Flow Regimes	474
6.11.2	Knudson-Flow-Regime Surface Accommodation and Slip Coefficients	476
6.11.3	Slip Coefficients in Transitional-Flow Regime	480
6.11.4	Solid Particle Thermophoresis in Gases	481
6.11.5	Physical Adsorption and Desorption	482
6.11.6	Disjoining Pressure in Ultrathin-Liquid Films	486
6.12	Turbulent-Flow Structure and Boundary-Layer Transport	487
6.12.1	Turbulent Kinetic Energy Spectrum for Homogeneous Turbulence	489
6.12.2	Boundary-Layer Turbulent Heat Flux	491
6.12.3	Turbulent Mixing Length and Turbulent Thermal Conductivity	492
6.12.4	Spatial Variation of Boundary-Layer Turbulent Mixing Length	493
6.12.5	Turbulent Mixing Using Lagrangian Langevin Equation	494

6.13	Thermal Plasmas: Plasma Thermal Conductivity	494
6.13.1	Free Electron Density and Plasma Thermal Conductivity	496
6.13.2	Thermal Nonequilibrium Plasma Energy Equation	500
6.13.3	Species Concentrations for Two-Temperature Plasmas	501
6.13.4	Kinetics of Energy Exchange Between Electrons and Heavier Species	501
6.14	Size Effects	502
6.14.1	Effective Thermal Conductivity in Gas-Filled Narrow Gaps	502
6.14.2	Thermal Creep (Slip) Flow in Narrow Gaps	508
6.15	Problems	511
<b>7</b>	<b>Photon Energy Storage, Transport, and Transformation Kinetics . . . .</b>	<b>519</b>
7.1	Quantum-Particle Treatment: Photon Gas and Blackbody Emission	523
7.2	Lasers and Near-Field (EM Wave) Thermal Emission	527
7.2.1	Lasers and Narrow-Band Emissions	527
7.2.2	Classical EM Wave Near-Field Thermal Emission	528
7.3	Quantum and Semiclassical Treatments of Photon-Matter Interaction	529
7.3.1	Hamiltonians of Radiation Field	530
7.3.2	Photon-Matter Interactions	533
7.4	Photon Absorption and Emission in Two-Level Electronic Systems	534
7.4.1	Einstein Excited-State Population Rate Equation	535
7.4.2	Einstein Coefficients for Equilibrium Electronic Population	537
7.4.3	Spontaneous Versus Stimulated Emissions in Equilibrium Thermal Cavity $f_{ph}^o$	538
7.4.4	Spectral Absorption Coefficient and Cross-Section Area	539
7.5	Particle Treatment: Photon BTE with Absorption, Emission, and Scattering	541
7.5.1	Combining Absorption and Emission	543
7.5.2	Photon-Free Electron Elastic Scattering Rate and Cross-Section Area	544
7.6	Photon Intensity: Equation of Radiative Transfer	547
7.6.1	General Form of ERT	547
7.6.2	Optically Thick Limit, Mean Free Path, and Radiant Conductivity	549
7.7	Wave Treatment: Field Enhancement and Photon Localization	552
7.7.1	Photon Localization in One-Dimensional Multilayer	552

## Contents

xv

7.7.2	Coherence and Electric Field Enhancement	556
7.7.3	Comparison with Particle Treatment (ERT)	558
7.8	Continuous and Band Photon Absorption	562
7.8.1	Photon Absorption Coefficient for Solids	562
7.8.2	Photon Absorption Coefficient for Gases	567
7.9	Continuous and Band Photon Emission	571
7.9.1	Emission Mechanisms	571
7.9.2	Absorption and Emission Reciprocity (Kirchhoff Law)	572
7.10	Spectral Surface Emissivity	574
7.11	Radiative and Nonradiative Decays and Quantum Efficiency	577
7.12	Anti-Stokes Fluorescence: Photon–Electron–Phonon Couplings	582
7.12.1	Anti-Stokes Laser Cooling (Phonon Absorption) of Ion-Doped Solids	582
7.12.2	Laser Cooling Efficiency	584
7.12.3	Photon–Electron–Phonon Transition Rate Using Weak Coupling Approximation	587
7.12.4	Time Scales for Laser Cooling of Solids (Weak Couplings)	592
7.12.5	Optimal Host Material	596
7.12.6	Photon–Electron and Electron–Phonon Transition Rates Using Strong Couplings ( <i>Ab Initio</i> Computation)	598
7.13	Gas Lasers and Laser Cooling of Gases	608
7.13.1	Molecular-Gas Lasers	608
7.13.2	Laser Doppler Cooling of Atomic Gases and Doppler Temperature	627
7.14	Photovoltaic Solar Cell: Reducing Phonon Emission	631
7.14.1	Single-Bandgap Ideal Solar PV Efficiency	634
7.14.2	Multiple-Bandgap Ideal Solar PV Efficiency	636
7.14.3	Semiempirical Solar PV Efficiency	639
7.15	Size Effects	642
7.15.1	Enhanced Near-Field Radiative Heat Transfer	642
7.15.2	Photon Energy Confinement by Near-Field Optical Microscopy	645
7.15.3	Hot Phonon Recycling in Photonics	646
7.16	Problems	650
APPENDIX A: Tables of Properties and Universal Constants . . . . .		661
APPENDIX B: Derivation of Green–Kubo Relation . . . . .		668
APPENDIX C: Derivation of Minimum Phonon Conductivity Relations . . .		676
APPENDIX D: Derivation of Phonon Boundary Resistance . . . . .		683

APPENDIX E: Derivation of Fermi Golden Rule . . . . .	689
APPENDIX F: Derivation of Equilibrium, Particle Probability Distribution Functions . . . . .	696
APPENDIX G: Phonon Contributions to the Seebeck Coefficient . . . . .	701
APPENDIX H: Monte Carlo Method for Carrier Transport . . . . .	709
APPENDIX I: Ladder Operators . . . . .	713
<i>Nomenclature</i>	719
<i>Abbreviations</i>	725
<i>Glossary</i>	727
<i>Bibliography</i>	741
<i>Index</i>	765



## Preface

Heat is atomic motion of matter, and temperature indicates the equilibrium distribution of this motion. Nonequilibrium atomic motions, created for example by a temperature gradient, result in heat transfer. Heat transfer physics describes the thermodynamics and kinetics (mechanisms and rates) of energy storage, transport, and transformation by means of principal energy carriers. Heat is energy that is stored in the temperature-dependent motion and within the various particles that make up all matter in all of its phases, including electrons, atomic nuclei, individual atoms, and molecules. Heat can be transferred to and from matter by one or more of the principal energy carriers: electrons<sup>†</sup> (either as classical or quantum entities), fluid particles (classical particles or quantum particles), phonons (lattice-vibration quantum waves, i.e., quasi-particles), and photons<sup>‡</sup> (quantum particles). The state of the energy stored within matter or transported by the carriers can be described by a combination of classical and quantum statistical mechanics. The energy is also transformed (converted) between the various carriers. All processes that act on this energy are ultimately governed by the rates at which various physical phenomena occur, such as the rate of particle collisions in classical mechanics. It is the combination of these various processes (and their governing rates) within a particular system that determines the overall system behavior, such as the net rate of energy storage or transport. Controlling every process, from the atomic level (studied here) to the macroscale (covered in an introductory heat transfer course), are the laws of thermodynamics, including conservation of energy.

The focus of this text is on the heat transfer behavior (the storage, transport, and transformation of thermal energy) of the aforementioned principal energy carriers at the atomic scale. The specific mechanisms are described in detail, including elastic/inelastic collisions/scattering among particles, quasi-particles, and waves. Particular attention is given to the time scales over which energy transport or

<sup>†</sup> For semiconductors, the holes are included as energy carriers. For electrolytes, ion transport is treated similarly.

<sup>‡</sup> Here, *photon* refers to both the classical (Maxwell) and the quantum (quasi-particle, Schrödinger) descriptions of the electromagnetic waves.

transformation processes occur, so that the reader gains some sense of how they compare with one another, as well as how they combine to produce overall system energy storage–transport–transformation rates. The approach taken here begins with a survey of fundamental concepts of atomic-level physics. This survey includes a look at the energy within the electronic states of atoms, as well as interatomic forces and potentials. Various theories of molecular dynamics and transport are also described. After this overview, in-depth, quantitative analyses are performed for each of the principal energy carriers, including analysis of how they interact with each other. This combination should allow for the teaching of a thorough introduction of heat transfer physics within one semester, without prolonged preparation or significant prerequisites. In general, several areas of physics are relevant to the study of heat transfer: (a) atomic–molecular dynamics, (b) solid state (condensed matter), (c) electromagnetism, and (d) quantum optics. No prior knowledge of these areas is necessary to appreciate the material of this text (a knowledge of introductory heat transfer is assumed).

Crystalline solids and their vibrational and electronic energies are treated first. This discussion is followed by an examination of energies of fluid particles and their interactions with solid surfaces. Then the interactions of photons with matter are posed with photons as EM waves, as particles, or as quasi-particles.

The text is divided into seven chapters, starting with the introduction and preliminaries of Chapter 1, in which the microscale carriers are introduced and the scope of the heat transfer physics is defined. Chapter 2 is on molecular electronic orbitals, interatomic and intermolecular potentials, molecular dynamics, and an introduction to quantum energy states. Chapter 3 is on microscale energy transport and transition kinetics theories, including the Boltzmann transport equation, the Maxwell equations, the Langevin stochastic transport equation, the Onsager coupled transport relation, and the Green–Kubo fluctuation–dissipation transport coefficients and relations. Chapters 4, 5, 6, and 7 cover the transport and interactions of phonons, electrons, fluid particles, and photons, respectively.

The size effects (where the system size affects the atomic-level behavior) on transport and energy conversion, for each principal carrier, are considered at the ends of Chapters 4 to 7. This allows for reference to applications in nanostructured and microstructured systems.

Some of the essential derivations are given as appendices. Appendix B gives the Green–Kubo relation, Appendix C gives the minimum phonon conductivity relations, Appendix D gives the phonon boundary resistance, Appendix E gives the Fermi Golden Rule, and Appendix F gives the particle energy distribution (occupancy) functions for bosons (phonons and photons), fermions (electrons), and Maxwell–Boltzmann (fluid) particles. Appendix G is on contributions to the Seebeck coefficient from various charge-carrier interactions, including with phonons. Appendix H is on the Monte Carlo method used for the simulation of energy carrier transport. Appendix I is on the ladder operators used for the carrier state transition by creation (raising) and annihilation (lowering).

Some end-of-chapter problems are provided to enhance understanding and familiarity and to allow for specific calculations. When needed, computer programs are also used. A full, digital solutions manual is available.

In general, vectors (lowercase) and tensors (uppercase) are in bold type. A nomenclature, an abbreviations list, and a glossary of relevant terms are given at the end of the text. Numbers in parenthesis indicate equation numbers. The periodic table of elements, with the macroscopic (bulk) and atomic properties, is given in Appendix A (in Tables A.1 and A.2), along with the tables of the universal and derived constants and unit prefixes.

It is hoped that this treatment provides an idea of the scope and some of the fundamentals of heat transfer physics, along with some of the most recent findings in the field.

Massoud Kaviany  
Ann Arbor  
kaviany@umich.edu

Cambridge University Press  
978-1-107-04178-3 - Heat Transfer Physics: Second Edition  
Massoud Kaviany  
Frontmatter  
[More information](#)

---

## Acknowledgments

Many doctoral students and postdoctoral Fellows working with me have contributed to this book. Among them are Jae Dong Chung, Luciana da Silva, Baoling Huang, Gi Suk Hwang, Dan Johnson, Ankur Kapoor, Hyoungchul Kim, Jedo Kim, Scott Gayton Liter, Alan McGaughey, Corey Melnick, Da Hye Min, Brendan O'Connor, Xiulin Ruan, Seungha Shin, and Xiangchun Zhang. Alan, Baoling, Corey, Gayton, Gi Suk, Hyoungchul, Seungha, and Xiulin have provided many ideas and have been constant sources of inspiration. I am indebted to all of them; without them this task could not have been completed. I would also like to thank the National Science Foundation (Thermal Transport and Processes) and the Department of Energy (Basic Energy Sciences) for sponsoring the research leading to some of the materials presented here.