# Low-energy Charged Particles in Atomic and Molecular Gases

# Michael A. Morrison, R. E. Robson, and R. D. White

# Contents

Version 2.12: February 13, 2006

# Preface

- 1. INTRODUCTION
  - A. Motivation for studying charged particles in gases: applications to science and technology
  - B. Swarms vs plasmas
  - C. Historical survey of theory and experiment
  - D. Theme: microscopic collision properties reflected in macroscopic transport properties
  - E. Outline of contents
- 2. EXPERIMENTAL CONSIDERATIONS AND APPLICATIONS
  - A. Measurement vs theory
  - B. Single-scattering beam experiments
  - C. Drift-tube experiments: time-of-flight, steady-state Townsend, Cavallieri, and Frank-Hertz
  - D. Gas discharges and plasma processing
  - E. Other applications: multi-wire drift chambers, muon-catalyzed fusion

# Part A: Foundations–Microscopic Considerations

# 3. COLLISIONS IN ATOMIC AND MOLECULAR GASES

- A. Low-energy scattering processes and their cross sections
- B. Characteristic behavior of low-energy cross sections
- C. Threshold laws
- D. Modified effective-range theory for atoms and molecules
- E. Simple parameter-dependent models of near-threshold cross sections for use in transport analysis
- 4. ESSENTIALS OF COLLISION THEORY
  - A. Quantum-mechanical definitions of cross sections and other fundamental scattering quantities
  - B. Time-reversal and parity invariance and their consequences for cross sections
  - C. The electron-target interaction potential
  - D. Effects of constituents of the interaction potential on low-energy cross sections
  - E. The special role of the point charge-induced dipole interaction
  - F. Boundary conditions and scattering quantities
  - G. Quantum-mechanical description of collision dynamics: scattering from a central potential
  - H. Quantum-mechanical description of collision dynamics: scattering from a non-central potential
  - I. Quantum-mechanical description of collision dynamics: scattering from an atom
  - J. Quantum-mechanical description of collision dynamics: scattering from a molecule
  - K. Special phenomena in low-energy collisions: resonances, virtual states, Ramsauer-Townsend minima
  - L. The relationship between particle-particle cross sections and quantities measured in crossed-beam experiments
- 5. COLLISIONS BETWEEN HEAVY PARTICLES
  - A. Classical treatment of ions: from interaction potentials to cross sections
  - B. The impact-parameter representation
  - C. The semi-classical description of a collision

#### 6. ESSENTIAL ATOMIC STRUCTURE FOR LOW-ENERGY COLLISIONS

- A. Qualitative atomic structure: the shell model
- B. Characteristic values of quantities that describe atoms in their ground states
- C. An overview of the quantum mechanics of atomic structure I: the independent-particle model
- D. Atomic orbitals and the limitations of the shell model
- E. An overview of the quantum mechanics of atomic structure II: beyond the independent-particle model
- F. Electron correlation in atoms
- G. Excited, metastable, and Rydberg states of atoms
- H. Energy levels and spectra of atomic ions
- I. Negative ions
- J. Atoms in external fields
- 7. ESSENTIAL MOLECULAR STRUCTURE FOR LOW-ENERGY COLLISIONS
  - A. The Born-Oppenheimer approximation and its limitations
  - B. Electronic states of molecules in the Born-Oppenheimer approximation
  - C. Molecular symmetry for diatomic and polyatomic molecules
  - D. Classification and term symbols for electronic states of molecules
  - E. Born-Oppenheimer potential energies and their limitations
  - F. The Franck-Condon approximation
  - G. Rovibrational states of molecules in the Born-Oppenheimer approximation
  - H. Molecular properties: spectroscopic constants and polarizabilities
  - I. Characteristic values of quantities that describe low-lying electronic states of molecules and their rotational, and vibrational energy levels
  - J. Dissociation, ionization, and related rearrangement processes in molecules
  - K. Molecular orbitals and their conceptual limitations
  - L. Electron correlation in molecules
  - M. Beyond the Born-Oppenheimer approximation: "exact" molecular structure
  - N. Molecules in external fields

### 8. ELECTRON-ATOM SCATTERING: PHYSICS AND CHARACTERISTIC EXAMPLES

- A. A closer look at the Schrödinger equation and boundary conditions
- B. The Born and distorted-wave approximations
- C. Variational methods
- D. Eigenfunction expansion methods
- E. The role of exchange, correlation, and polarization
- F. Characteristic features of elastic integral and differential cross sections
- G. Examples of resonance phenomena, threshold behavior, and Ramsauer-Townsend minima

#### 9. ELECTRON-MOLECULE SCATTERING: PHYSICS AND CHARACTERISTIC EXAMPLES

- A. A closer look at the Schrödinger equation and boundary conditions
- B. Elastic scattering
- C. Momentum transfer cross sections
- D. Rotational excitation
- E. Vibrational excitation
- F. Dissociative and other rearrangement processes
- G. Characteristic features of elastic integral and differential cross sections for various electron-molecule scattering processes

## Part B: Foundations-Macroscopic Considerations

#### 10. KINETIC THEORY: BRIDGING THE MICROSCOPIC-MACROSCOPIC GAP

- A. The role of kinetic theory in statistical mechanics
- B. Phase space, distribution functions, moments, the mean free path, cross section, and collision rate
- C. Collision moments for an arbitrary quantity
- D. The Boltzmann equation: derivation and assumptions
- E. The H-theorem, the Maxwellian distribution of velocities
- F. The Fokker-Planck equation, Lorentz gas, Rayleigh gas
- G. Charge exchange, the collision operator in the relaxation-time model
- H. Inelastic collisions, the Wang-Chang et al. semiclassical collision operator, the Maxwell-Boltzmann distribution of internal states, finite-difference formulation for light particles
- I. Quantum kinetic equations (Waldmann-Snider) for a Fermi-Dirac gas and for a Bose-Einstein gas

### 11. THE HYDRODYNAMIC REGIME AND TRANSPORT COEFFICIENTS

- A. Moment equations
- B. The hydrodynamic regime; density gradient expansion
- C. Transport coefficients: definitions, and reaction rates
- D. The hierarchy of hydrodynamic kinetic equations
- E. The diffusion equation and its solution for various experimental arrangements
- F. Non-hydrodynamic situations
- 12. MATHEMATICAL AND NUMERICAL METHODS
  - A. Tensor structure and geometrical symmetries
  - B. Orthogonal-function expansions
  - C. Representation of Boltzmanns equation
  - D. Burnett-function representations of Boltzmanns equation
  - E. The collision matrix, the Talmi transformation
  - F. Discrete-ordinate representations
  - G. Variational methods

## Part C: Analytic and Approximate Calculations

#### 13. MODEL KINETIC EQUATION SOLUTIONS

- A. Why use models?
- B. Exact transport coefficients for the constant-collision-frequency model
- C. Exact analytic solution of a model kinetic equation for hydrodynamic and non-hydrodynamic regimes in the time-of-flight experiment
- D. Exact analytic solution for the kinetic equation in the idealized charge-exchange model in a radio-frequency field
- 14. MOMENTUM TRANSFER THEORY AND APPLICATIONS
  - A. Approximation of the collision moments
  - B. The Wannier energy relation
  - C. Ficks law and the generalized Einstein relations
  - D. Blancs law for gas mixtures
  - E. Negative differential conductivity
  - F. Tonks theorem and the equivalent field approximation
  - G. Radio frequency fields; the effective field

# 15. REACTIVE EFFECTS

- A. Balance equations with reactive terms
- B. Attachment and ionization cooling
- C. Reactive corrections to transport properties: the two types of transport coefficients

### 16. FLUID MODELING OF PLASMAS AND SWARMS

- A. The need for consistency with the swarm limit
- B. Use of swarm data in plasma models
- C. Ambipolar diffusion
- D. Fluid modeling of stead-state Townsend and Franck-Hertz experiments

## Part D: Numerical Calculations and Applications

### 17. SOLUTION OF BOLTZMANN EQUATION FOR LIGHT CHARGED PARTICLES

- A. Energy exchange; the spherical-harmonic representation in speed space
- B. The Lorentz gas, the "two-term" approximation, and the need for a "multi-term" theory
- C. Examples of hydrodynamic transport coefficients and distribution functions:  $e^--CH_4$ ,  $e^--H_2O$ ,  $e^+-Ar$ , muon-deuterium, etc.
- D. Reactive effects
- E. Crossed electric and magnetic fields
- F. Time-varying fields; anomalous anisotropic diffusion
- G. The Franck-Hertz experiment
- 18. BOUNDARY CONDITIONS, TRANSPORT PROPERTIES AND DIFFUSION COOLING
  - A. General comments on boundary conditions
  - B. The Cavalleri experiment and diffusion cooling
  - C. The eigenvalue problem for zero field
  - D. The variational method
  - E. Diffusion cooling with an alternating electric field
  - F. Concluding remarks

## 19. ION TRANSPORT

- A. Historical review
- B. The importance of having a unified approach for ions and electrons
- C. Two- and three-temperature theories
- D. The mass-ratio expansion
- E. Selected examples

### 20. FURTHER APPLICATIONS

- A. Hot-atom chemistry
- B. Muon catalyzed fusion
- C. Positrons in gases
- D. Oddities: negative absolute mobility, countergradient flow

# Part E: Back to Atomic and Molecular Physics

- 21. DETERMINATION OF CROSS SECTIONS AND INTERACTION POTENTIALS FROM TRANSPORT DATA
  - A. The importance of determining charged-particle cross sections
  - B. The importance of swarm data
  - C. Inversion methods
  - D. Uniqueness problems

# Appendices

- A. Data resources for cross sections
- B. Summary of vector calculus
- C. Summary of tensors and dyadics
- D. Summary of non-relativistic quantum mechanics for bound and scattering states
- E. List of symbols
- F. Physical constants, units, and conversion factors

# Bibliography

Index