



Spectral Methods in Chemistry and Physics: Applications to Kinetic Theory and Quantum Mechanics (Scientific Computation)

Bernard Shizgal

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This book is a pedagogical presentation of the application of spectral and pseudospectral methods to kinetic theory and quantum mechanics. There are additional applications to astrophysics, engineering, biology and many other fields. The main objective of this book is to provide the basic concepts to enable the use of spectral and pseudospectral methods to solve problems in diverse fields of interest and to a wide audience. While spectral methods are generally based on Fourier Series or Chebychev polynomials, non-classical polynomials and associated quadratures are used for many of the applications presented in the book. Fourier series methods are summarized with a discussion of the resolution of the Gibbs phenomenon. Classical and non-classical quadratures are used for the evaluation of integrals in reaction dynamics including nuclear fusion, radial integrals in density functional theory, in elastic scattering theory and other applications. The subject matter includes the calculation of transport coefficients in gases and other gas dynamical problems based on spectral and pseudospectral solutions of the Boltzmann equation. Radiative transfer in astrophysics and atmospheric science, and applications to space physics are discussed. The relaxation of initial non-equilibrium distributions to equilibrium for several different systems is studied with the Boltzmann and Fokker-Planck equations.

The eigenvalue spectra of the linear operators in the Boltzmann, Fokker-Planck and Schrödinger equations are studied with spectral and pseudospectral methods based on non-classical orthogonal polynomials. The numerical methods referred to as the Discrete Ordinate Method, Differential Quadrature, the Quadrature Discretization Method, the Discrete Variable Representation, the Lagrange Mesh Method, and others are discussed and compared.

MATLAB codes are provided for most of the numerical results reported in the book - see Link under 'Additional Information' on the the right-hand column.

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