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Nota di contenuto	Multidimensional Quantum Dynamics; Contents; Preface; List of Contributors; List of Symbols; 1 Introduction; Part 1 Theory; 2 The Road to MCTDH; 2.1 The Standard Method; 2.2 Time-Dependent Hartree; 3 Basic MCTDH Theory; 3.1 Wavefunction Ansatz and Equations of Motion; 3.2 The Constraint Operator; 3.3 Efficiency and Memory Requirements; 3.4 Multistate Calculations; 3.5 Parametrized Basis Functions: G-MCTDH; 4 Integration Schemes; 4.1 The Variable Mean-Field (VMF) Integration Scheme; 4.2 A Simple Constant Mean-Field (CMF) Integration Scheme; 4.3 Why CMF Works; 4.4 Second-Order CMF Scheme 5 Preparation of the Initial Wavepacket5.1 Initial Wavepacket as Hartree Product; 5.2 Eigenstates and Operated Wavefunctions; 6 Analysis of the Propagated Wavepacket; 6.1 Runtime Analysis of Accuracy; 6.2 Spectra; 6.2.1 Photoabsorption Spectra; 6.2.2 Eigenvalues and Filter Diagonalization; 6.2.3 Time-Resolved Spectra; 6.3 Optimal Control; 6.4 State Populations; 6.5 Reaction Probabilities; 7 MCTDH for Density

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12.2.2.2 Introduction of the Body-Fixed Frame and Quantization

12.2.3 Introduction of the Body-Fixed Projections of the Angular Momenta Associated With the $N - 1$ Vectors; 12.3 General Expression of KEO in Standard Polyspherical Coordinates; 12.3.1 General Expression; 12.3.1.1 Definition of the BF frame: Figure 12.3; 12.3.1.2 Polyspherical Parametrization; 12.3.1.3 Properties of the BF Projections of the Angular Momenta; 12.3.1.4 General Expression of the KEO in Polyspherical Coordinates; 12.3.1.5 Introduction of a Primitive Basis Set of Spherical Harmonics; 12.4 Examples

12.4.1 Scattering Systems: $H(2) + H(2)$

Sommario/riassunto

The first book dedicated to this new and powerful computational method begins with a comprehensive description of MCTDH and its theoretical background. There then follows a discussion of recent extensions of MCTDH, such as the treatment of identical particles, leading to the MCTDHF and MCTDHB methods for fermions and bosons. The third section presents a wide spectrum of very different applications to reflect the large diversity of problems that can be tackled by MCTDH. The result is handbook and ready reference for theoretical chemists, physicists, chemists, graduate students, lecturers and