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Nota di contenuto	BEYOND BORN-OPPENHEIMER; CONTENTS; PREFACE; ABBREVIATIONS; 1 MATHEMATICAL INTRODUCTION; 1.1 Hilbert Space; 1.1.1 Eigenfunction and Electronic Nonadiabatic Coupling Term; 1.1.2 Abelian and Non-Abelian Curl Equations; 1.1.3 Abelian and Non-Abelian Divergence Equations; 1.2 Hilbert Subspace; 1.3 Vectorial First-Order Differential Equation and Line Integral; 1.3.1 Vectorial First-Order Differential Equation; 1.3.1.1 Study of Abelian Case; 1.3.1.2 Study of Non-Abelian Case; 1.3.1.3 Orthogonality; 1.3.2 Integral Equation; 1.3.2.1 Integral Equation along an Open Contour 1.3.2.2 Integral Equation along a Closed Contour 1.3.3 Solution of Differential Vector Equation; 1.4 Summary and Conclusions; Problem; References; 2 BORN-OPPENHEIMER APPROACH: DIABATIZATION AND TOPOLOGICAL MATRIX; 2.1 Time-Independent Treatment; 2.1.1 Adiabatic Representation; 2.1.2 Diabatic Representation; 2.1.3 Adiabatic-to-Diabatic Transformation; 2.1.3.1 Transformation for Electronic Basis Sets; 2.1.3.2 Transformation for Nuclear

Wavefunctions; 2.1.3.3 Implications Due to Adiabatic-to-Diabatic Transformation; 2.1.3.4 Final Comments; 2.2 Application of Complex Eigenfunctions
2.2.1 Introducing Time-Independent Phase Factors 2.2.1.1 Adiabatic Schrodinger Equation; 2.2.1.2 Adiabatic-to-Diabatic Transformation; 2.2.2 Introducing Time-Dependent Phase Factors; 2.3 Time-Dependent Treatment; 2.3.1 Time-Dependent Perturbative Approach; 2.3.2 Time-Dependent Nonperturbative Approach; 2.3.2.1 Adiabatic Time-Dependent Electronic Basis Set; 2.3.2.2 Adiabatic Time-Dependent Nuclear Schrodinger Equation; 2.3.2.3 Time-Dependent Adiabatic-to-Diabatic Transformation; 2.3.3 Summary; Problem; 2A Appendixes; 2A.1 Dressed Nonadiabatic Coupling Matrix
2A.2 Analyticity of Adiabatic-to-Diabatic Transformation Matrix A in Spacetime ConfigurationReferences; 3 MODEL STUDIES; 3.1 Treatment of Analytical Models; 3.1.1 Two-State Systems; 3.1.1.1 Adiabatic-to-Diabatic Transformation Matrix; 3.1.1.2 Topological (D) Matrix; 3.1.1.3 The Diabatic Potential Matrix; 3.1.2 Three-State Systems; 3.1.2.1 Adiabatic-to-Diabatic Transformation Matrix; 3.1.2.2 Topological Matrix; 3.1.3 Four-State Systems; 3.1.3.1 Adiabatic-to-Diabatic Transformation Matrix; 3.1.3.2 Topological Matrix; 3.1.4 Comments Related to General Case
4.3 Quantization of Nonadiabatic Coupling Matrix: Study of Ab Initio Molecular Systems

Sommario/riassunto

INTRODUCING A POWERFUL APPROACH TO DEVELOPING RELIABLE QUANTUM MECHANICAL TREATMENTS OF A LARGE VARIETY OF PROCESSES IN MOLECULAR SYSTEMS. The Born-Oppenheimer approximation has been fundamental to calculation in molecular spectroscopy and molecular dynamics since the early days of quantum mechanics. This is despite well-established fact that it is often not valid due to conical intersections that give rise to strong nonadiabatic effects caused by singular nonadiabatic coupling terms (NACTs). In Beyond Born-Oppenheimer, Michael Baer, a leading authority on molecular scattering theory an
