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2.2.1 Introducing Time-Independent Phase Factors2.2.1.1 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