Scientific Publications of Robert E. Wyatt

1. A. L. Companion and R. E. Wyatt, The Diffuse Reflectance Spectra of Titanium Oxides, *J. Phys. Chem. Solids* **24**, 1025 (1963).
2. R. E. Wyatt and R. G. Parr, One-Electron Perturbations in Self-Consistent Field Theory, *J. Chem. Phys.* **41**, 514 (1964).
3. R. E. Wyatt and R. G. Parr, Origin of the Barrier Hindering Internal Rotation in Ethane, *J. Chem. Phys.* **41**, 3262 (1964).
4. R. E. Wyatt and R. G. Parr, Theory of the Origin of the Barrier Hindering Internal Rotation in the Ethane Molecule I, *J. Chem. Phys.* **43**, 5217 (1965).
5. R. E. Wyatt and R. G. Parr, Theory of the Origin of the Barrier Hindering Internal Rotation in the Ethane Molecule II, *J. Chem. Phys.* **44**, 1529 (1966).
6. R. E. Wyatt, H. F. King, R. E. Stanton, and R. G. Parr, Corresponding Orbitals and the Nonorthogonality Problem in Molecular Quantum Mechanics, *J. Chem. Phys.* **47**, 1936 (1967).
7. S. Epstein, A. C. Hurley, R. E. Wyatt and R. G. Parr, Integrated and Integral Hellman-Feynman Theorems, *J. Chem. Phys.* **47**, 1275 (1967).
8. E. A. McCullough, Jr. and R. E. Wyatt, Quantum Dynamics of the Collinear (H, H_2) Reaction, *J. Chem. Phys.* **51**, 1253 (1969).
9. R. E. Wyatt, Quantum Dynamics of the H + H_2 Reaction: Investigation of Vibrational Adiabatic Models, *J. Chem. Phys.* **51**, 3489 (1969).
10. J. L. Jackson and R. E. Wyatt, Fast Determination of Resonance States in Atomic Collisions, *Chem. Phys. Lett.* **4**, 643 (1970).
11. E. A. McCullough, Jr. and R. E. Wyatt, Dynamics of the Collinear H + H_2 Reaction I: Probability Density and Flux, *J. Chem. Phys.* **54**, 3578 (1971).
12. E. A. McCullough, Jr. and R. E. Wyatt, Dynamics of the Collinear H + H_2 Reaction II: Energy Analysis, *J. Chem. Phys.* **54**, 3592 (1971).
13. J. L. Jackson and R. E. Wyatt, Quantum Effects in Transient Pair Formation in Gases: The Equilibrium Constant for O + H → OH*, *J. Chem. Phys.* **54**, 5271 (1971).
14. R. E. Wyatt, Theory of Three-Dimensional Chemical Reactions Using Natural Collision Coordinates, *J. Chem. Phys.* **56**, 390 (1972).
15. P. B. Middleton and R. E. Wyatt, Broken Path Model of Reactive Collisions: Application to Collinear H + H_2, *J. Chem. Phys.* **56**, 2702 (1972).
16. R. B. Walker and R. E. Wyatt, DWBA Study of the Collinear H + H_2 Reaction, *Chem. Phys. Lett.* **16**, 52 (1972).
17. S. H. Harms and R. E. Wyatt, Natural Bifurcation Coordinates for Three-Dimensional Chemical Reactions, *J. Chem. Phys.* **57**, 2722 (1972).
18. R. B. Walker and R. E. Wyatt, Hindered Rotor States for the Planar H + H_2 Reaction, *J. Chem. Phys.* **57**, 2728 (1972).
19. P. B. Middleton and R. E. Wyatt, Quantum Mechanical Study of a Reaction Path Bifurcation Model, *Chem. Phys. Lett.* **21**, 57 (1973).
20. J. L. Jackson and R. E. Wyatt, H_3 Potential Energy Surface in Natural Collision Coordinates, *Chem. Phys. Lett.* **18**, 161 (1973).
21. R. B. Walker and R. E. Wyatt, Three-Dimensional Reaction Cross Sections from Planar Scattering Data, *Mol. Phys.* **28**, 101 (1974).
22. R. B. Walker and R. E. Wyatt, DWBA Study of the Planar H + H_2 Reaction, *J. Chem. Phys.* 61, 4839 (1974).
23. S. H. Harms and R. E. Wyatt, Hindered Asymmetric Top States for Chemical Reactions, *J. Chem. Phys.* **62**, 3162 (1975).
24. S. H. Harms and R. E. Wyatt, Hindered Asymmetric Top Wavefunctions for Three Dimensional H + H_2, *J. Chem. Phys.* **62**, 3173 (1975).
25. A. B. Elkowitz and R. E. Wyatt, Approximate Hindered Asymmetric Top Wavefunctions for Atom-Diatomic Molecule Reactions, *J. Chem. Phys.* **62**, 3682 (1975).
26. A. B. Elkowitz and R. E. Wyatt, Quantum Mechanical Reaction Cross Sections for the Three Dimensional Hydrogen Exchange Reaction, *J. Chem. Phys.* **62**, 2504 (1975).
27. A. B. Elkowitz and R. E. Wyatt, Three Dimensional Natural Coordinate Asymmetric Top Theory of Reactions: Application to H + H_2, *J. Chem. Phys.* **63**, 702 (1975).
28. M. J. Redmon and R. E. Wyatt, Three Dimensional Quantum Mechanical Studies of the H + H_2 and F + H_2 Reactions, *Int. J. Quantum Chem. Symp.* **9**, 403 (1975).
29. R. E. Wyatt, Information Theoretic Analysis of Quantum Mechanical Reaction Cross Sections, *Chem. Phys. Lett.* **34**, 167 (1975).
30. S. H. Harms, A. B. Elkowitz and R. E. Wyatt, Asymmetric Top States for Chemical Reactions, *Mol. Phys.* **31**, 177 (1976).
31. A. B. Elkowitz and R. E. Wyatt, J_z-conserving Approximation for the Hydrogen Exchange Reaction, *Mol. Phys.* **31**, 189 (1976).
32. D. L. Miller and R. E. Wyatt, Comparison of Diatomics in Molecules and Simple Valence Bond Potential Energy Surfaces for F + H_2, *Chem. Phys. Lett.* **38**, 410 (1976).
33. D. G. Truhlar and R. E. Wyatt, History of H_3 Kinetics, *Annu. Rev. Phys. Chem.* **27**, 1 (1976).
34. J. McNutt, S. Latham, M. J. Redmon, and R. E. Wyatt, Comment on Resonance Structure in the Collinear H + H_2 Reaction, *Discuss. Faraday Soc.* **62**, 322 (1976).
35. D. L. Miller and R. E. Wyatt, Electronuclear Basis for Three-Dimensional Electronic Nonadiabiatic Chemical Reactions, *J. Chem. Phys.* **67**, 1302 (1977).
36. M. J. Redmon and R. E. Wyatt, Computational Methods for Reactive Scattering, *Int. J. Quantum Chem. Symp.* **11**, 343 (1977).
37. D. G. Truhlar and R. E. Wyatt, H + H_2: Potential Energy Surfaces and Elastic and Inelastic Scattering, *Adv. Chem. Phys.* **36**, 141 (1977).
38. R. E. Wyatt, Quantum Mechanics of Neutral Atom-Diatom Reactions, in P. R. Brooks and E. F. Hayes (Eds.), State-to-State Chemistry, *ACS Symp. Ser.* **56**, 185 (1977).

10.1021/jp0795412
Published on Web 10/11/2007

39. J. F. McNutt, S. L. Latham, R. E. Wyatt, and M. J. Redmon, Quantum Dynamics of the F + H_2 Reaction: Resonance Models, and Probability Density and Flux Distributions, *J. Chem. Phys.* **69**, 3746 (1978).
40. R. E. Wyatt, Reactive Scattering Cross Sections: Approximate Quantal Treatments, in R. Bernstein (Ed.), *Atom-Molecule Collision Theory: A Guide for the Experimentalist* (Plenum, New York, 1979), Ch. 8b.
41. R. E. Wyatt, Direct Mode Reactions: Methodology for Accurate Quantal Calculations, in R. Bernstein (Ed.), *Atom-Molecule Collision Theory: A Guide for the Experimentalist* (Plenum, New York, 1979), Ch. 9a.
42. J. F. McNutt, and R. E. Wyatt, Generalized Hyperbolic Coordinates for Collinear Reactive Scattering, *J. Chem. Phys.* **70**, 5307 (1979).
43. R. B. Walker and R. E. Wyatt, Quantum Mechanics of Electronic-Rotational Energy Transfer in F(^{2}P) + H_2 Collisions, *J. Chem. Phys.* **70**, 1601 (1979).
44. S. Leasure and R. E. Wyatt, Sequential vs. Direct Multiphoton Absorption, *Chem. Phys. Lett.* **61**, 626 (1079).
45. M. J. Redmon and R. E. Wyatt, Quantum Resonance Structure in the Three Dimensional F + H_2 Reaction, *Chem. Phys. Lett.* **63**, 209 (1979).
46. R. E. Wyatt, Quantum Mechanical Study of F($^2P_{1/2}$) + H_2($j = 0$) Quenching, *Chem. Phys. Lett.* **63**, 503 (1979).
47. J. F. Hutchinson and R. E. Wyatt, Detailed Dynamics of Collinear F + H_2 Trajectories, *J. Chem. Phys.* **70**, 3509 (1979).
48. R. T. Penley, J. F. Hutchinson and R. E. Wyatt, Pattern Prediction in Collinear Atom-Diatom Trajectories, *Chem. Phys. Lett.* **69**, 255 (1980).
49. S. C. Leasure and R. E. Wyatt, Floquet Theory of the Interaction of a Molecule with a Laser Field: Techniques and an Application, *Opt. Eng.* **19**, 46 (1980).
50. J. F. Hutchinson and R. E. Wyatt, Quantum Ergodicity and the Wigner Distribution, *Chem. Phys. Lett.* **72**, 384 (1980).
51. S. C. Leasure and R. E. Wyatt, Sudden Rotation Approximation for Non-Resonant Transitions in an Intense Laser Field, *J. Chem. Phys.* **73**, 4439 (1980).
52. R. E. Wyatt, Quantum Mechanical Study of Chemical Reaction Dynamics, in K. Fukui and B. Pullman (Eds.), *Horizons of Quantum Chemistry* (Reidel, Dordrecht, 1980), p. 63.
53. J. F. McNutt and R. E. Wyatt, Comparison of Close-Coupling and Approximate Methods for F($^2P_{1/2}$) + H_2 Non-Reactive Collisions, *Chem. Phys.* **58**, 423 (1981).
54. S. C. Leasure, K. F. Milfeld, and R. E. Wyatt, Quantum Molecular Dynamics in Intense Laser Fields: Theory and Applications to Diatomic Molecules, *J. Chem. Phys.* **74**, 6197 (1981).
55. C. L. Shoemaker and R. E. Wyatt, Feshback Resonances in Chemical Reactions, in P. O. Lowdin (Ed.), *Adv. Quantum Chem.* **14**, 169 (1981).
56. J. F. Hutchinson and R. E. Wyatt, Quantum Ergodicity for Time-Dependent Wave Packet Dynamics, *Phys. Rev. A* **23**, 1567 (1981).
57. J. F. McNutt and R. E. Wyatt, Quantum Dynamics of the Three Dimensional F + H_2 Reaction: Wavefunction Density Analysis, in D. G. Truhlar (Ed.), *Potential Energy Surfaces and Dynamics Calculations* (Plenum, New York, 1981), p. 495.
58. E. Pollak, J. F. McNutt, and R. E. Wyatt, Density and Flux Analysis for the Collinear H + H_2 Reaction, *Chem. Phys.* **70**, 207 (1982).
59. D. Martin and R. E. Wyatt, Classical Dynamics of Multiphoton Dissociation for a Model System, *Chem. Phys.* **64**, 203 (1982).
60. M. J. Davis and R. E. Wyatt, Surface-of-Section Analysis in the Classical Theory of Multiphoton Absorption, *Chem. Phys. Lett.* **86**, 235 (1982).
61. R. E. Wyatt, J. F. McNutt, and M. J. Redmon, Analysis of the Resonance in the Three Dimensional F + H_2 Reaction, *Ber. Bunsen-Ges. Phys. Chem.* **86**, 437 (1982).
62. C. Leforestier and R. E. Wyatt, Time-Dependent Semiclassical *R*-Matrix Theory of Multiphoton Dissociation, *Phys. Rev. A* **25**, 1250 (1982).
63. C. L. Shoemaker and R. E. Wyatt, Computational Approach to the Green Function in Reactive Scattering, *J. Chem. Phys.* **76**, 1347 (1982).
64. C. L. Shoemaker and R. E. Wyatt, Theory of Resonances in Three Dimensional Chemical Reactions I. Feshbach Analysis and Computational Techniques, *J. Chem. Phys.* **77**, 4982 (1982).
65. C. L. Shoemaker and R. E. Wyatt, Theory of Resonances in Three Dimensional Chemical Reactions II. Application to a Model Atom-Diatom Reaction, *J. Chem. Phys.* **77**, 4994 (1982).
66. E. Pollak and R. E. Wyatt, Semiclassical Prediction of Resonance Energies in Three Dimensional Reactive Collisions, *J. Chem. Phys.* **77**, 3689 (1982).
67. M. J. Davis, R. E. Wyatt, and C. Leforestier, Classical and Quantum Mechanical Studies of Molecular Excitation and Dissociation, in J. Jortner and B. Pullman (Eds.), *Intramolecular Dynamics* (Reidel, Dordrecht, 1980), p. 403.
68. K. F. Milfeld and R. E. Wyatt, Study, Extension, and Application of Floquet Theory for Quantum Molecular Systems in an Oscillating Field, *Phys. Rev. A* **27**, 72 (1983).
69. E. Pollak and R. E. Wyatt, Semiclassical Prediction of Adiabatic Barriers on a Three Dimensional Potential Energy Surface, *J. Chem. Phys.* **78**, 4464 (1983).
70. R. E. Wyatt, G. Hose, and H. Taylor, Mode-Selective Multiphoton Excitation of a Model System, *Phys. Rev. A* **28**, 915 (1983).
71. M. J. Redmon and R. E. Wyatt, Quantum Mechanical Differential Reaction Cross Sections for the F + H_2($v = 0$) → FH($v = 2,3$) + H Reaction, *Chem. Phys. Lett.* **96**, 284 (1983).
72. M. Mohan, K. F. Milfeld, and R. E. Wyatt, Laser Assisted Chemical Reactions: Semiclassical Approach Employing Floquet and R-Matrix Theories, *Chem. Phys. Lett.* **99**, 411 (1983).
73. S. L. Ding and R. E. Wyatt, Time-Independent Energy Sudden Transformation, *J. Chem. Phys.* **78**, 5637 (1983).
74. C. Leforestier and R. E. Wyatt, Optical Potential for Laser Induced Dissociation, *J. Chem. Phys.* **78**, 2334 (1983).
75. R. F. Nalewajski and R. E. Wyatt, Collisional Perturbation of Regular and Irregular Intramolecular Dynamics: A Classical Study, *Chem. Phys.* **81**, 357 (1983).
76. A. Nauts and R. E. Wyatt, A New Approach to Many State Quantum Dynamics: The Recursive Residue Recursion Method, *Phys. Rev. Lett.* **51**, 2238 (1983).

77. E. Pollak and R. E. Wyatt, Adiabatic-Sudden Transition in Chemical Reactions: Study of a Model for $H + H_2$-($v = 1$), *Chem. Phys. Lett.* **110**, 340 (1984).
78. E. Pollak and R. E. Wyatt, Semiclassical Adiabatic Theory of Resonances in Chemical Reactions: Application to 3D $H + H_2$ and $F + H_2$, *J. Chem. Phys.* **81**, 1801 (1984).
79. R. F. Nalewajski and R. E. Wyatt, Collisional Perturbation of Regular and Irregular Intramolecular Dynamics: A Model Quantum Mechanical Study, *Chem. Phys.* **85**, 117 (1984).
80. R. F. Nalewajski and R. E. Wyatt, Collisional Perturbation of Regular and Irregular Intramolecular Dynamics: State-to-State Study of a Model, *Chem. Phys.* **89**, 385 (1984).
81. J. F. McNutt, R. E. Wyatt, and M. J. Redmon, Quantum Mechanical Study of the Three Dimensional $F + H_2$ Reaction I. Energy Partitioning and Entropy Analysis in the Collision Complex, *J. Chem. Phys.* **81**, 1692 (1984).
82. J. F. McNutt, R. E. Wyatt, and M. J. Redmon, Quantum Mechanical Study of the Three Dimensional $F + H_2$ Reaction II. Density and Flux Analysis in the Collision Complex, *J. Chem. Phys.* **81**, 1794 (1984).
83. C. C. Marston and R. E. Wyatt, Resonant Quasiperiodic and Periodic Orbits for the 3D $F + H_2$ Reaction, in D. G. Truhlar (Ed.), *Resonances in Electron-Molecule, van der Waals Complexes, and Reactive Chemical Dynamics* (*ACS Symp. Ser.* **263**, 1984), p. 441.
84. A. Nauts, A. R. E. Wyatt, Theory of Laser-Molecule Interaction: The Recursive Residue Generation Method, *Phys. Rev. A* **30**, 872 (1984).
85. C. C. Marston and R. E. Wyatt, Semiclassical Theory of Resonances in 3D Chemical Reactions I. Resonant Periodic Orbits for $F + H_2$, *J. Chem. Phys.* **81**, 1819 (1984).
86. C. C. Marston and R. E. Wyatt, Semiclassical Theory of Resonances in 3D Chemical Reactions II. Resonant Quasiperiodic Oribts for $F + H_2$, *J. Chem. Phys.* **83**, 3390 (1985).
87. C. C. Marston, R. C. Brown, and R. E. Wyatt, Semiclassical Wavepacket Construction of Quantum Resonance States From Classical Resonant Orbits for the $F + H_2$ Reaction, *Chem. Phys. Lett.* **122**, 205 (1985).
88. K. F. Milfeld and R. E. Wyatt, Quantum Mechanical Study of Multiphoton Excitation of the Nonrotating OCS Molecule, *J. Chem. Phys.* **83**, 1457 (1985).
89. K. F. Milfeld, J. E. Castillo, and R. E. Wyatt, Dynamics of Eigenstate Transitions Induced by External Fields: A New Approach, *J. Chem. Phys.* **83**, 1617 (1985).
90. J. E. Castillo and R. E. Wyatt, Recursive Residue Generation Method for Laser Molecule Interaction: Utilization of Structured Sparsity, *J. Comput. Phys.* **59**, 120 (1985).
91. C. Leforestier and R. E. Wyatt, Role of Feshback Resonances in the Infrared Multiphoton Dissociation of Small Molecules, *J. Chem. Phys.* **82**, 752 (1985).
92. C. Leforestier and R. E. Wyatt, Infrared Multiphoton Dissociation Calculation of a Model Linear Triatomic, *Chem. Phys.* **98**, 123 (1985).
93. J. Chang, S. L. Ding, and R. E. Wyatt, Theory of Multiphoton Excitation of Methane in Intense Laser Fields, *J. Chem. Phys.* **83**, 3244 (1985).
94. R. C. Brown and R. E. Wyatt, Vibrational Resonances and IR Multiphoton Excitation, *J. Chem. Phys.* **82**, 4777 (1985).
95. I. Schek and R. E. Wyatt, Generation and Interpretation of Chain Parameters in the Recursive Residue Generation Method, *J. Chem. Phys.* **83**, 3028 (1985).
96. I. Schek and R. E. Wyatt, Diagrammatic Representation in the Recursive Residue Generation Method: Multiphoton Excitation of an Active Mode Coupled to a Molecular Background, *J. Chem. Phys.* **83**, 4650 (1985).
97. M. Page, E. S. Oran, J. P. Boris, D. Miller, R. E. Wyatt, H. Rabitz, and B. A. Waite, A Comparison of Quantum, Classical, and Semiclassical Descriptions of a Model Collinear Inelastic Collision of Two Diatomic Molecules, *J. Chem. Phys.* **83**, 5635 (1985).
98. R. E. Wyatt, Direct Computation of Quantal Rate Constants: Recursive Development of the Flux Autocorrelation Function, *Chem. Phys. Lett.* **121**, 301 (1985).
99. B. op de Haar, G. G. Balint-Kurti, and R. E. Wyatt, An Approximate Three Dimensonal Quantum Mechanical Calculation of Reactive Scattering Cross Sections for the $H + Cl_2 \rightarrow HCl + Cl$ Reaction, *J. Phys. Chem.* **89**, 4007 (1985).
100. C. C. Marston, R. C. Brown, and R. E. Wyatt, Semiclassical Wavepacket Construction of Quantum Resonance States from Classical Resonant Orbits for the $F + H_2$ Reaction, *Chem. Phys. Lett.* **122**, 205 (1985).
101. C. Leforestier and R. E. Wyatt, Infrared Multiphoton Dissociation of a Model Linear Triatomic, *Chem. Phys.* **98**, 123 (1985).
102. J. Chang and R. E. Wyatt, Artificial Intelligence Techniques in the Study of Multiphoton Dynamics: Application to a General Vibrating-Rotating Spherical Top Molecule, *Chem. Phys. Lett.* **121**, 307 (1985).
103. J. Chang and R. E. Wyatt, Preselecting Paths for Multiphoton Dynamics Using Artificial Intelligence, *J. Chem. Phys.* **85**, 1826 (1986).
104. J. Chang and R. E. Wyatt, Influence of Rotational States on Molecular Multiphoton Excitation, *J. Chem. Phys.* **85**, 1840 (1986).
105. J. Chang, N. Moiseyev, and R. E. Wyatt, Stable Highly Excited Vibrational Eigenvalues without the Variational Principle, *J. Chem. Phys.* **84**, 4997 (1986).
106. R. A. Friesner, R. E. Wyatt, C. Hempel, and B. Criner, A Generalized Version of the Recursive Residue Generation Method for Vector Computers, *J. Comput. Phys.* **64**, 220 (1986).
107. R. E. Wyatt and D. Scott, Quantum Dynamics with the Recursive Residue Method: Improved Algorithm for Chain Propagators, in J. Cullum and R. Willoughby (Eds.), *Large Scale Eigenvalue Problems* (North Holland, Amsterdam, 1986), p. 67.
108. I. Schek and R. E. Wyatt, Importance of Linked Diagrams in the Recursive Residue Generation Method, *J. Chem. Phys.* **84**, 4497 (1986).
109. I. Schek and R. E. Wyatt, Time-Evolution in Multi-State Quantal Systems: Use of Irreducible Moments, *Chem. Phys. Lett.* **129**, 99 (1986).
110. I. Schek and R. E. Wyatt, Generation and Importance of Linked and Irreducible Moment Diagrams in the Recursive Residue Generation Method, in Y. Prior, A. Ben-Reuven, and M. Rosenbluh (Eds.), *Methods of Laser Spectroscopy* (Plenum, New York, 1986), p. 347.

111. R. C. Brown and R. E. Wyatt, Quantum Mechanical Manifestation of Cantori: Wavefunction Localization in the Stochastic Region, *Phys. Rev. Lett.* **57**, 1 (1986).
112. R. C. Brown and R. E. Wyatt, Barriers to Chaotic Classical Motion and Quantum Mechanical Localization in Multiphoton Dissociation, *J. Phys. Chem.* **90**, 3590 (1986).
113. N. Moiseyev, R. C. Brown, R. E. Wyatt, and E. Tzidoni, Analysis of Chaotic Eigenfunctions by the Natural Expansion Method, *Chem. Phys. Lett.* **127**, 37 (1986).
114. N. Moiseyev and R. E. Wyatt, Natural Expansion of Vibrational Wavefunctions: RRGM with Residue Algebra, *Chem. Phys. Lett.* **132**, 396 (1986).
115. N. Moiseyev, R. A. Friesner, and R. E. Wyatt, Natural Expansion of Multi-Mode Vibrational Wavefunctions, *J. Chem. Phys.* **85**, 331 (1986).
116. D. L. Miller and R. E. Wyatt, Quantum Dynamics of the Three-Dimensional Li + HF Reaction: The Bending Corrected Rotating Nonlinear Model, *J. Chem. Phys.* **86**, 5557 (1987).
117. D. L. Miller and R. E. Wyatt, Differential Reaction Cross Sections in the Bending Corrected Rotating Nonlinear Model: Li + HF → LiF + H, *Chem. Phys. Lett.* **133**, 126 (1987).
118. R. E. Wyatt, Quantum Dynamics on the Cray-XMP, in E. Wimmer (Ed.) *Computational Chemistry on Cray Supercomputers* (Cray Research Inc, Mendota Heights, MN, 1987), p. 57.
119. I. Schek and R. E. Wyatt, Effect of Diagonal and Off-Diagonal Disorder in the Multiphoton Excitation of an Active Mode Couled to a Bath, in R. Lefebvre and S. Mukamel (Eds.), *Stochasticity and Intramolecular Redistribution of Energy* (Reidel, Dordrecht, 1987), p. 95.
120. R. A. Friesner, J. P. Brunet, R. E. Wyatt, and C. Leforestier, Computational Approach to Large Quantum Dynamical Problems, *Int. J. Supercomputer Appl. and High Perform. Comput.* **1**, 9 (1987).
121. I. Schek, N. Moiseyev, and R. E. Wyatt, Quantum Mechanical Study of the Survival Probability in Laser Driven Molecules: The Role of Diagonal and Off-Diagonal Disorder, *Phys. Rev. A* **36**, 3743 (1987).
122. C. Duneczky and R. E. Wyatt, Multilevel Adaptive Technique for Quantum Reactive Scattering, *J. Chem. Phys.* **87**, 4519 (1987).
123. R. E. Wyatt, Time Dependent Quantum Mechanics on Supercomputers, in R. B. Wilhelmson (Ed.), *High Speed Computing: Scientific Applications and Algorithm Design* (University of Illinois Press, Urbana, 1988), p. 166.
124. J. P. Brunet, C. Leforestier, and R. E. Wyatt, Quantum Correlations in a Model for Multiple-Photon Absorption, *J. Chem. Phys.* **88**, 3125 (1988).
125. J. P. Brunet, R. A. Friesner, R. E. Wyatt, and C. Leforestier: Theoretical Study of the IR Absorption-Spectrum of HCN, *Chem. Phys. Lett.* **153**, 425 (1988).
126. J. P. Brunet, R. E. Wyatt, H. S. Taylor, and J. Zakrzewski, Time Evolution in a Driven Quantum System: Excitation Through Bands of States, *Phys. Rev. A* **38**, 5602 (1988).
127. C. Duneczky and R. E. Wyatt, Lanczos Recursion, Continued Fractions, Pade Approximants, and Variational Principles in Quantum Scattering Theory, *J. Chem. Phys.* **89**, 1448 (1988).
128. C. Duneczky and R. E. Wyatt, Recursive Generation of Individual *S*-Matrix Elements: Application to Inelastic Collisions, *J. Phys. B* **21**, 3727 (1988).
129. M. Dmello, C. Duneczky, and R. E. Wyatt, Recursive Generation of Individual S-Matrix Elements: Application to the Collinear H + H_2 Reaction, *Chem. Phys. Lett.* **148**, 169 (1988).
130. R. F. Nalewajski, J. Korchowiec, and R. E. Wyatt, Effect of Basis Set Non-Orthogonality in the Wigner R-Matrix Theory of Scattering, *Acta Phys. Pol., A* **74**, 269 (1988).
131. I. Schek and R. E. Wyatt, Discretization of a Continuum Coupled to a Discrete State by Tridiagonalizing the Schrodinger Equation, *J. Chem. Phys.* **89**, 4924 (1988).
132. B. Ramachandran, T. G. Wei, and R. E. Wyatt, The Role of Basis Set Expansions in the Relative Performance of the Schwinger and Newton Variational Principles, *Chem. Phys. Lett.* **151**, 540 (1988).
133. B. Ramachandran, T. G. Wei, and R. E. Wyatt, Relative Performances of the Kohn, Schwinger, and Newton Variational Principles in Scattering Theory, *J. Chem. Phys.* **89**, 6785 (1988).
134. D. E. Manolopoulos and R. E. Wyatt, Quantum Scattering via the Log Derivative Version of the Kohn Variational Principle, *Chem. Phys. Lett.* **152**, 23 (1988).
135. C. Duneczky, R. E. Wyatt, D. Chatfield, K. Haug, D. W. Schwenke, D. G. Truhlar, Y. Sun, and D. J. Kouri, Iterative Methods for Solving the Non-Sparse Equations of Quantum Mechanical Reactive Scattering, *Comput. Phys. Commun.* **53**, 357 (1989).
136. B. Ramachandran and R. E. Wyatt, How Variational Methods in Scattering Theory Work, in A. Lagana (Ed.), *Supercomputer Algorithms for Reactivity, Dynamics, and Kinetics of Small Molecules* (Klauder Academic Publishers, 1989), p. 169.
137. B. Ramachandran and R. E. Wyatt, The Schwinger and Newton Variational Principles for the Log Derivative Matrix, *J. Chem. Phys.* **91**, 1096 (1989).
138. C. C. Marston and R. E. Wyatt, Semiclassical Cluster Model for Wave Propagation in Molecular Crystals, *Chem. Phys. Lett.* **162**, 386 (1989).
139. R. E. Wyatt, Quantum Dynamics with Thousands of States: Applications to Laser-Molecule Interaction, Spectroscopy, and Scattering Theory, *Comments At. Mol. Phys.* **22**, 185 (1989).
140. J. A. Bentley, J. P. Brunet, R. E. Wyatt, R. A. Friesner, and C. Leforestier, Quantum Mechanical Study of the SEP Spectrum for HCN, *Chem. Phys. Lett.* **161**, 393 (1989).
141. D. E. Manolopoulos and R. E. Wyatt, Calculations Relating to the Experimental Observation of Resonances in the H + H_2 Reaction, *Chem. Phys. Lett.* **159**, 123 (1989).
142. D. E. Manolopoulos, M. Dmello, and R. E. Wyatt, Quantum Reactive Scattering via the Log Derivative Version of the Kohn Variational Principle: General Theory for Bimolecular Chemical Reactions, *J. Chem. Phys.* **91**, 6096 (1989).
143. D. L. Boley, L. A. Collins, Y. Saad, D. G. Truhlar, and R. E. Wyatt, Practical Iterative Methods for Large-Scale Computations, *Comp. Phys. Commun.* **53**, R11 (1989).
144. D. E. Manolopoulos and R. E. Wyatt, H + $H_2(0,0)$ → $H_2(v', j')$ + H Integral Cross Sections on the Double Many Body Expansion Potential Energy Surface, *J. Chem. Phys.* **92**, 810 (1990).
145. M. M. Budhikot, B. F. Womak, and R. E. Wyatt, Circuit Simulation of Signal Propagation in the Neuron, *Proc. Comput. Sim. Conf.*, 1989.

146. T. M. Flosnik and R. E. Wyatt, Complex Effective Hamiltonian Approach for IR Multiphoton Dissociation, *Phys. Rev. A* **40**, 5716 (1989).

147. J. O. Hirschfelder, R. E. Wyatt, and R. D. Coalson (Eds.), Lasers, Molecules, and Methods, *Adv. Chem. Phys.* 1989.

148. R. E. Wyatt, The Recursive Residue Method, in J. O. Hirschfelder, R. E. Wyatt, and R. D. Coalson (Eds.), Lasers, Molecules, and Methods, *Adv. Chem. Phys.* 1989.

149. M. Dmello, D. E. Manolopoulos, and R. E. Wyatt, Converged Variational Quantum Scattering Results for the 3-Dimensional F + D_2 Reaction, *Chem. Phys. Lett.* **168**, 113 (1990).

150. D. E. Manolopoulos, R. E. Wyatt, and D. C. Clary, Iterative Solution in Quantum Scattering Theory: The Log Derivative Kohn Approach, *J. Chem. Soc., Faraday Trans.* **86**, 1641 (1990).

151. D. E. Manolopoulos, M. Dmello, R. E. Wyatt, and R. B. Walker, Converged Variational Quantum Scattering Results for the 3-Dimensional F + HD Reaction, *Chem. Phys. Lett.* **169**, 482 (1990).

152. D. E. Manolopoulos, M. Dmello, and R. E. Wyatt, Translational Basis Set Contraction in Variational Reactive Scattering, *J. Chem. Phys.* **93**, 403 (1990).

153. M. Mohan, K. F. Milfeld, and R. E. Wyatt, A New General *R*-Matrix Theory of Collinear Reactions and its Application to the H + H_2 Reaction, *Mol. Phys.* **70**, 1085 (1990).

154. E. Thomas, P. Patton, and R. E. Wyatt, Computational Dynamics of Signal Propagation in the Visual Cortex, *Proceedings of the Cray Users Group*, 1990, p. 22.

155. B. Ramachandran, M. Dmello, and R. E. Wyatt, The Newton Variational Functional for the Log-Derivative Matrix: Use of the Reference Energy Green Function in an Exchange Problem, *J. Chem. Phys.* **93**, 8110 (1990).

156. E. Thomas, P. Patton, and R. E. Wyatt, A Computational Model of the Vertical Anatomical Organization of Primary Visual Cortex, *Bio. Cyber.* **65**, 189 (1991).

157. R. E. Wyatt and J. W. Driver, Computational Brain Dynamics: Visualization of Activity Flow in the Cerebral Cortex, *Cray Channels*, **Fall**, 24 (1991).

158. M. Witten and R. E. Wyatt, Neural Orchestration: From Cortical Simulation to Cortical Symphony, *Proc. USENIX Conference*, Nashville (1991).

159. J. S. Wright, R. J. Williams, and R. E. Wyatt, The F + H_2 → HF + H Reaction: Classical and Quantum Reaction Dynamics on a New Collinear ab initio Surface, *Chem. Phys. Lett.* **184**, 159 (1991).

160. M. Dmello, D. E. Manolopoulos, and R. E. Wyatt, Quantum Dynamics of the H + D_2 → D + HD Reaction: Comparison with Experiment, *J. Chem. Phys.* **94**, 5985 (1991).

161. J. Chang, N. J. Brown, M. Dmello, R. E. Wyatt, and H. Rabitz, Quantum Functional Sensitivity Analysis for the Collinear H + H_2 Reaction, *J. Chem. Phys.* **96**, 3523 (1992).

162. P. Patton, E. Thomas, and R. E. Wyatt, A Computational Model of Vertical Signal Propagation in the Primary Visual Cortex, *Bio. Cyber.* **68**, 43 (1992).

163. R. E. Wyatt, C. Lung, and C. Leforestier, Quantum Dynamics of Overtone Relaxation in Benzene.1. 5-Mode and 9-Mode Models for Relaxation from CH($n = 3$), *J. Chem. Phys.* **97**, 3458 (1992).

164. R. E. Wyatt, C. Lung, and C. Leforestier, Quantum Dynamics of Overtone Relaxation in Benzene. 2. 16 Mode Model for Relaxation from CH($n = 3$), *J. Chem. Phys.* **97**, 3477 (1992).

165. T. G. Wei and R. E. Wyatt, Semiclassical Dynamics of Shock Wave Propagation and Energy Redistribution among Vibrational Modes in a Morse Molecular Lattice, *J. Phys. Chem. Solids* **53**, 871 (1992).

166. M. Witten and R. E. Wyatt, Increasing our Understanding of Biological Models through Visual and Sonic Representations: A Cortical Case Study, *Int. J. Supercomput. Appl.* **6**, 257 (1992).

167. J. Chang, N. J. Brown, M. D'Mello, R. E. Wyatt, and H. Rabitz, Quantum Functional Sensitivity Analysis within the Log-Derivative Kohn Variational Method for Reactive Scattering, *J. Chem. Phys.* **97**, 6226 (1992).

168. J. Chang, N. J. Brown, M. D'Mello, R. E. Wyatt, and H. Rabitz, Predicting Observables on Different Potential Energy Surfaces using Feature Sensitivity Analysis: Application to the Collinear H + H_2 Exchange Reaction, *J. Chem. Phys.* **97**, 6240 (1992).

169. J. A. Bentley, R. E. Wyatt, M. Menou, and C. Leforestier, A Finite Basis-Discrete Variable Representation Calculation of Vibrational Levels of Planar Acetylene, *J. Chem. Phys.* **97**, 4255 (1992).

170. J. S. Wright, M. Kolbuszewski, and R. E. Wyatt, Multireference Configuration Interaction Potential Surfaces for the Collinear F + H_2 Reaction, *J. Chem. Phys.* **97**, 8296 (1992).

171. T. G. Wei and R. E. Wyatt, Analytical Potential Surface for the HFCO → HF + CO Unimolecular Reaction, *J. Phys. Chem.* **97**, 13580 (1993).

172. X. D. Wu, B. Ramachandran, and R. E. Wyatt, A Single Arrangement Variational Method for Total Reaction Probabilities, *Chem. Phys. Lett.* **214**, 118 (1993).

173. L. J. Brenner, J. Senekowitsch, and R. E. Wyatt, Coupled Cluster Calculation of the Inplane Harmonic Force Field of Benzene, *Chem. Phys. Lett.* **215**, 63 (1993).

174. R. E. Wyatt and C. Iung, Quantum Dynamics of Overtone Relaxation in Benzene. 3. Spectra and Dynamics for Relaxation from CH($v = 3$), *J. Chem. Phys.* **98**, 5191 (1993).

175. R. E. Wyatt and C. Iung, Quantum Dynamics of Overtone Relaxation in Benzene. 4. Relaxation from CH($v = 4$), *J. Chem. Phys.* **98**, 3577 (1993).

176. R. E. Wyatt and C. Iung, Quantum Dynamics of Overtone Relaxation in Benzene .5. CH($v = 3$) Dynamics Computed with a New ab initio Force Field, *J. Chem. Phys.* **98**, 6758 (1993).

177. C. Iung and R. E. Wyatt, Time Dependent Quantum Mechanical Study of Intramolecular Vibrational Energy Redistribution in Benzene, *J. Chem. Phys.* **99**, 2261 (1993).

178. C. Lung, C. Leforestier, and R. E. Wyatt, Wave Operator and Artificial Intelligence Contraction Algorithms in Quantum Dynamics: Application to CD_3H and C_6H_6, *J. Chem. Phys.* **98**, 6722 (1993).

179. J. A. Bentley, C. M. Huang, and R. E. Wyatt, Highly-Vibrationally Excited HCN- HNC Eigenvalues, Wave-Functions, and Stimulated-Emission Pumping Spectra, *J. Chem. Phys.* **98**, 5207 (1993).
180. X. D. Wu, R. E. Wyatt, and M. D'Mello, Inclusion of the Geometric Phase in Quantum Reactive Scattering Calculations: A Variational Formulation, *J. Chem. Phys.* **101**, 2953 (1994).
181. X. D. Wu, B. Ramachandran, and R. E. Wyatt, A Single Arrangement Variational Method for Reactive Scattering: Total and State-Resolved Reaction Probabilities, *J. Chem. Phys.* **101**, 9395 (1994).
182. R. E. Wyatt, Quantum Dynamical Study of Intramolecular Dynamics and Spectroscopy, *Proc. Robert A. Welch Foundation 38th Conference on Chemical Research*, 1994, p. 113.
183. C. Leforestier and R. E. Wyatt, Computation of SEP Spectra, in H. Dai and R. W. Field (Eds.), *Molecular Dynamics and Spectroscopy by Stimulated Emission Pumping* (World Scientific, 1994), p. 755.
184. G. H. Yao and R. E. Wyatt, Stationary Approaches for Solving the Schrodinger Equation with Time-Dependent Hamiltonians, *J. Chem. Phys.* **101**, 1904 (1994).
185. M. J. D'Mello, D. E. Manolopoulos, and R. E. Wyatt, Theory, Experiment, and the H + D_2 Reaction, *Science* **263**, 102 (1994).
186. F. J. Aoiz, L. Banares, M. J. Dmello, V. J. Herrero, V. S. Rabanos, L. Schnieder, and R. E. Wyatt, Quantum Mechanical and Quasi-Classical Calculations for the H + D_2 → HD + D Reaction: Reaction Probabilities and Differential Cross Sections, *J. Chem. Phys.* **101**, 5781 (1994).
187. L. Schnieder, K. Seekamprahn, J. Borkowski, E. Wrede, K. H. Welge, F. J. Aoiz, L. Banares, M. J. Dmello, V. J. Herrero, V. S. Rabanos, and R. E. Wyatt, Experimental Studies and Theoretical Predictions for the H + D_2 → HD + D Reaction, *Science* **269** , 207 (1995).
188. G. H. Yao and R. E. Wyatt, A Krylov Subspace Chebyschev Method and its Application to Pulsed Laser Molecule Interaction, *Chem. Phys. Lett.* **239**, 207 (1995).
189. R. E. Wyatt, C. Iung, and C. Leforestier, Toward ab initio Intramolecular Dynamics, *Acc. Chem. Res.* **28**, 423 (1995).
190. R. E. Wyatt, Matrix Spectroscopy: Computation of Interior Eigenstates of Large Matrices using Layered Iteration, *Phys. Rev. E* **51**, 3643 (1995).
191. R. E. Wyatt, Computation of High-Energy Vibrational Eigenstates: Application to C_6H_5D, *J. Chem. Phys.* **103**, 8433 (1995).
192. A. T. Maynard, R. E. Wyatt, and C. Iung, A Quantum Dynamical Study of CH Overtones in Fluoroform. I. A Nine-Mode ab initio Surface, Vibrational Dynamics, and Spectroscopy, *J. Chem. Phys.* **103**, 8372 (1995).
193. S. A. Schofield, P. G. Wolynes, and R. E. Wyatt, Computational Study of Many Dimensional Quantum Energy Flow: From Action Diffusion to Localization, *Phys. Rev. Lett.* **74**, 3720 (1995).
194. E. Thomas and R. E. Wyatt, A Computational Model of Spindle Oscillations, *Math. Comput. Simul.* **40**, 35 (1995).
195. S. A. Schofield, R. E. Wyatt, and P. G. Wolynes: Computational Study of Many-Dimensional Quantum Vibrational Energy Redistribution .1. Statistics of the Survival Probability, *J. Chem. Phys.* **105**, 940 (1996).
196. R. E. Wyatt and J. Z. H. Zhang, (Eds.), *Dynamics of Molecules and Chemical Reactions* (Marcel Decker, New York, 1996).
197. C. Iung and R. E. Wyatt, Quantum Dynamical Studies of Molecular Spectra and Dynamics, in R. E. Wyatt and J. Z. H. Zhang, (Eds.), *Dynamics of Molecules and Chemical Reactions* (Marcel Decker, New York, 1996).
198. B. Ramachandran, J. Senekowitsch, and R. E. Wyatt, A New Potential Surface for the Reaction O + HCl → OH + Cl, *J. Mol. Struct.: THEOCHEM* **388**, 57 (1996).
199. B. Ramachandran, J. Senekowitsch, and R. E. Wyatt, A Quasiclassical Trajectory Study of the Reaction O + HCl ($v = 2$, $j = 1,6,9$) → OH(v', j') + Cl on a New Potential Surface, *Chem. Phys. Lett.* **270**, 387 (1997).
200. S. A. Schofield and R. E. Wyatt, Computational Study of Many-Dimensional Quantum Vibrational Energy Redistribution .2. Statistics of the Spectrum with Dynamical Implications, *J. Chem. Phys.* **106**, 7047 (1997).
201. A. Maynard, R. E. Wyatt, and C. Iung, A Quantum Dynamical Study of CH Overtones in Fluoroform .2. Eigenstate Analysis of the v(CH) = 1 and v(CH) = 2 Regions, *J. Chem. Phys.* **106**, 9483 (1997).
202. T. J. Minehardt, J. D. Adcock, and R. E. Wyatt, Enhanced Matrix Spectroscopy: The Preconditioned Green-Function Block Lanczos Algorithm, *Phys. Rev. E* **56**, 4837 (1997).
203. C. S. Guiang and R. E. Wyatt, Quantum Dynamics with Lanczos Subspace Propagation: Application to a Laser-Driven Molecular System, *Int. J. Quantum Chem.* **67**, 273 (1998).
204. C. S. Guiang and R. E. Wyatt, Torsional Eigenvalues of the Water Trimer on Several ab initio Potential Surfaces, *Int. J. Quantum Chem.* **68**, 233 (1998).
205. T. C. Allison, B. Ramachandran, J. Senekowitsch, D. G. Truhlar, and R. E. Wyatt, Variational Transition State Theory Calculations of Thermal Rate Coefficients for the O + HCl Reaction, *J. Mol. Struct.: THEOCHEM* **454**, 307 (1998).
206. R. E. Wyatt, Quantum Mechanical Study of the CH($v =$ 2) Overtone in 30-Mode Benzene, *J. Chem. Phys.* **109**, 10732 (1998).
207. T. J. Minehardt and R. E. Wyatt, Quasi-Classical Dynamics of Benzene Overtone Relaxation on an ab initio Force Field: 30-Mode Models of Energy Flow and Survival Probability for CH($v = 2$), *Chem. Phys. Lett.* **295**, 373 (1998).
208. T. J. Minehardt and R. E. Wyatt, Quasiclassical Dynamics of Benzene Overtone Relaxation on an ab initio Force Field. I. Energy Flow and Survival Probabilities in Planar Benzene for CH($v = 2,3$), *J. Chem. Phys.* **109** , 8330 (1998).
209. J. D. Adcock, T. J. Minehardt, and R. E. Wyatt, Visualization of the Dynamics of Energy Flow in Benzene, *J. Mol. Graphics Modell.* **16**, 297 (1998).
210. T. J. Minehardt, J. D. Adcock, R. E. Wyatt, and C. Iung, Quasi-Classical and Quantum Dynamics of Benzene Overtone Relaxation: Early Time ($t \leq 240$ fs) Intramolecular Vibrational Energy Redistribution for CH($n =$

2) in a 15-Mode Model, *Chem. Phys. Lett.* **303**, 347 (1999).
211. T. J. Minehardt, J. D. Adcock, and R. E. Wyatt, Energy Partitioning and Normal Mode Analysis of IVR in 30-Mode Benzene: Overtone Relaxation for CH($n = 2$), *Chem. Phys. Lett.* **303**, 537 (1999).
212. T. J. Minehardt, J. D. Adcock, and R. E. Wyatt, Quantum Dynamics of Overtone Relaxation in 30-Mode Benzene: A Time-Dependent Local Mode Analysis for CH($n = 2$), *J. Chem. Phys.* **110**, 3326 (1999).
213. C. L. Lopreore and R. E. Wyatt, Quantum Wavepacket Dynamics with Trajectories, *Phys. Rev. Lett.* **82**, 5190 (1999).
214. R. E. Wyatt, Quantum Wavepacket Dynamics with Trajectories: Application to Reactive Scattering, *J. Chem. Phys.* **111**, 4406 (1999).
215. T. J. Minehardt and R. E. Wyatt, Quantum Dynamics of Intramolecular Vibrational Energy Redistribution for Initially Excited CC Ring Modes in 30-Mode Benzene, *Chem. Phys. Lett.* **312**, 485 (1999).
216. B. Ramachandran, E. A. Schrader, J. Senekowitsch, and R. E. Wyatt, Dynamics of the O + HCl reaction on the ^{3}A″ Electronic State: A New ab initio Potential Energy Surface, Quasi-Classical Trajectory Study, and Comparison to Experiment, *J. Chem. Phys.* **111**, 3862 (1999).
217. R. E. Wyatt, Quantum Wavepacket Dynamics with Trajectories: Wavefunction Synthesis Along Quantum Paths, *Chem. Phys. Lett.* **313**, 189 (1999).
218. A. Vijay, R. E. Wyatt, and G. D. Billing, Time propagation and Spectral Filters in Quantum Dynamics: A Hermite Polynomial Perspective, *J. Chem. Phys.* **111**, 10794 (1999).
219. H. Zhang, B. Ramachandran, J. Senekowitsch, and R. E. Wyatt, Determination of Spectroscopic Constants and Anharmonic Force-Fields for HOCl and DOCl Using Scaled External Correlation, *J. Mol. Struct.: THEOCHEM* **487**, 75 (1999).
220. R. E. Wyatt, D. J. Kouri, and D. K. Hoffman, Quantum Wave Packet Dynamics with Trajectories: Implementation with Distributed Approximating Functionals, *J. Chem. Phys.* **112**, 10730 (2000).
221. C. S. Guiang and R. E. Wyatt, Quantum Control of I_2 Wave Packet Localization in Solid Argon Matrix, *J. Chem. Phys.* **112**, 3580 (2000).
222. A. Vijay and R. E. Wyatt, Spectral Filters in Quantum Mechanics: A Measurement Theory Perspective, *Phys. Rev. E* **62**, 4351 (2000).
223. C. L. Lopreore and R. E. Wyatt, Quantum Wave Packet Dynamics with Trajectories: Reflections on a Downhill Ramp Potential, *Chem. Phys. Lett.* **325**, 73 (2000).
224. C. L. Lopreore and R. E. Wyatt, "Comment on 'Quantum Wave Packet Dynamics with Trajectories'"—Lopreore and Wyatt Reply, *Phys. Rev. Lett.* **85**, 895 (2000).
225. E. R. Bittner and R. E. Wyatt, Integrating the Quantum Hamilton−Jacobi Equation by Wavefront Expansion and Phase Space Analysis, *J. Chem. Phys.* **113**, 8888 (2000).
226. R. E. Wyatt and E. R. Bittner, Quantum Wavepacket Dynamics with Trajectories: Implementation with Adaptive Lagrangian Grids, *J. Chem. Phys.* **113**, 8898 (2000).
227. K. Na and R. E. Wyatt, Quantum Trajectories for Resonant Scattering, *Int. J. Quantum Chem.* **8**, 206 (2001).
228. R. E. Wyatt, C. L. Lopreore, and G. Parlant, Electronic Transitions with Quantum Trajectories, *J. Chem. Phys.* **114**, 5113 (2001).
229. R. E. Wyatt and K. Na, Quantum Trajectory Analysis of Multimode Subsystem-Bath Dynamics, *Phys. Rev. E* **65**, 13 (2002).
230. C. L. Lopreore and R. E. Wyatt, Electronic Transitions with Quantum Trajectories II, *J. Chem. Phys.* **116**, 1228 (2002).
231. R. E. Wyatt, Wavepacket Dynamics on Adaptive Moving Grids, *J. Chem. Phys.* **117**, 9569 (2002).
232. K. H. Hughes and R. E. Wyatt, Wavepacket Dynamics on Dynamically Adapting Grids: Application of the Equidistribution Principle, *Chem. Phys. Lett.* **366**, 336 (2002).
233. K. S. Na and R. E. Wyatt, Quantum Hydrodynamic Analysis of Decoherence: Quantum Trajectories and Stress Tensor, *Phys. Lett. A* **306**, 97 (2002).
234. R. E. Wyatt, Recent Applications of the Quantum Trajectory Method, in M. Mohan (Ed.) *Current Developments in Atomic, Molecular, and Chemical Physics* (Klauder/Academic, New York, 2003).
235. K. Na and R. E. Wyatt, Quantum Hydrodynamic Analysis of Decoherence, *Phys. Script.* **XX**, 1 (2003).
236. C. J. Trahan and R. E. Wyatt, Radial Basis Function Interpolation in the Quantum Trajectory Method: Optimization of the Multiquadric Shape Parameter, *J. Comput. Phys.* **185**, 27 (2003).
237. C. J. Trahan and R. E. Wyatt, An Arbitrary Lagrangian-Eulerian Approach to Solving the Quantum Hydrodynamic Equations of Motion: Equidistribution with "Smart" Springs, *J. Chem. Phys.* **228**, 4784 (2003).
238. R. E. Wyatt and E. R. Bittner, Using Quantum Trajectories and Adaptive Grids to Solve Quantum Dynamical Problems, *Comput. Sci. Eng.* **5**, 22 (2003).
239. C. J. Trahan, K. Hughes, and R. E. Wyatt, A New Method for Wave Packet Dynamics: Derivative Propagation Along Quantum Trajectories, *J. Chem. Phys.* **118**, 9911 (2003).
240. D. Babyuk, J. H. Frederick, and R. E. Wyatt, Hydrodynamic Analysis of Dynamical Tunneling, *J. Chem. Phys.* **119**, 6482 (2003).
241. C. J. Trahan and R. E. Wyatt, Evolution of Classical and Quantum Phase Space Distributions: A New Trajectory Approach for Phase Space Hydrodynamics, *J. Chem. Phys.* **119**, 7017 (2003).
242. K. H. Hughes and R. E. Wyatt, Wavepacket Dynamics on Arbitrary Lagrangian-Eulerian Grids: Application to an Eckart Barrier, *Phys. Chem. Chem. Phys.* **5**, 3985 (2003).
243. K. H. Hughes and R. E. Wyatt, Trajectory Approach to Dissipative Quantum Phase Space Dynamics: Application to Barrier Scattering, *J. Chem. Phys.* **120**, 4089 (2004).
244. D. Babyuk and R. E. Wyatt, Hybrid Adaptive Algorithm for Wave Packet Dynamics, *Chem. Phys. Lett.* **387**, 227 (2004).
245. C. J. Trahan and R. E. Wyatt, Classical and Quantum Phase Space Evolution: Fixed-Lattice and Trajectory Solutions, *Chem. Phys. Lett.* **385**, 280 (2004).
246. F. Sales-Mayor and Robert E. Wyatt, A Two-Stage Filter for Smoothing Multivariate Noisy Data on Unstructured Grids, *Computers and Mathematics with Applications* **47**, 877 (2004).

247. D. Babyuk and R. E. Wyatt, Application of the Covering Function Method in Quantum Hydrodynamics for Two-Dimensional Scattering Problems, *Chem. Phys. Lett.* **400**, 145 (2004).
248. D. Babyuk and R. E. Wyatt, Coping with the Node Problem in Quantum Hydrodynamics: The Covering Function Method, *J. Chem. Phys.* **121**, 9230 (2004).
249. C. J. Trahan, R. E. Wyatt, and B. Poirier, Multidimensional Quantum Trajectories: Application of the Derivative Propagation Method, *J. Chem. Phys.* **122**, 16104 (2005).
250. R. E. Wyatt, *Quantum Dynamics with Trajectories* (Springer, New York, 2005), p. 405.
251. R. E. Wyatt and D. Babyuk, Multidimensional Reactive Scattering with Quantum Trajectories, *Phys. Rev. E* **73**, 046701 (2006).
252. D. Babyuk and R. E. Wyatt, Multidimensional Reactive Scattering with Quantum Trajectories: Dynamics with 50-200 Vibrational Modes, *J. Chem. Phys.* **124**, 214109 (2006).
253. D. Babyuk and R. E. Wyatt, Multidimensional Reactive Scattering with Quantum Trajectories: Dynamics with Morse Vibrational Modes, *J. Chem. Phys.* **125**, 064112 (2006).
254. L. R. Pettey and R. E. Wyatt, Wave Packet Dynamics with Adaptive Grids: The Moving Boundary Truncation Method, *Chem. Phys. Lett.* **424**, 443 (2006).
255. B. A. Rowland and R. E. Wyatt, Local and Non-Local Force Analysis for Wigner Function Barrier Scattering, *Chem. Phys. Lett.* **426**, 209 (2006).
256. C.-C. Chou and R. E. Wyatt, Computational Method for the Quantum Hamilton−Jacobi Equation: Bound States in One-Dimension, *J. Chem. Phys.* **125**, 174103 (2006).
257. C.-C. Chou and R. E. Wyatt, Computational Method for the Quantum Hamilton-Jacobi Equation: One-Dimensional Scattering Problems, *Phys. Rev. E* **74**, 066702 (2006).
258. L. R. Pettey and R. E. Wyatt, Wave Packet Dynamics with Adaptive Grids: The Moving Boundary Truncation Method, *Chem. Phys. Lett.* **424**, 443 (2006).
259. L. R. Pettey and R. E. Wyatt, Quantum Wave Packet Dynamics on Multidimensional Adaptive Grids: Applications of the Moving Boundary Truncation Method, *Int. J. Quantum Chem.* **107**, 1566 (2007).
260. C.-C. Chou and R. E. Wyatt, Riccati Differential Equation for Quantum Mechanical Bound States: Comparison of Numerical Integrators, *Int. J. Quantum Chem.*, in press.
261. B. A. Rowland and R. E. Wyatt, Analysis of Barrier Scattering with Real and Complex Quantum Trajectories, *J. Phys. Chem. A* **41**, 10234 (2007).
262. R. E. Wyatt and B. A. Rowland, Quantum Trajectories in Complex Phase Space: Multi-Dimensional Barrier Scattering, *J. Chem. Phys.* **127**, 044103 (2007).
263. C.-C. Chou and R. E. Wyatt, Quantum Trajectories in Complex Space, *Phys. Rev. A* **76**, 012115 (2007).
264. R. E. Wyatt and C.-C. Chou, Ray−Wave Front Method for Solving the Multi-dimensional Quantum Hamiltonian Jacobi Equation, *Phys. Rev. A*, submitted for publication.
265. R. E. Wyatt and D. Babyuk, Frenet Frame Formulation of the Reaction Path Hamiltonian, *J. Chem. Phys.*, submitted for publication.
266. J. K. David and R. E. Wyatt, Barrier Scattering with Complex-Valued Quantum Trajectories: Taxonomy and Analysis of Isochrones, *J. Chem. Phys.*, submitted for publication.
267. B. A. Rowland and R. E. Wyatt, Complex Trajectories sans Isochrones: Quantum Barrier Scattering with Rectilinear Constant Velocity Trajectories, *J. Chem. Phys.*, in press.