# Publications of William H. Miller†

1. P. E. Eberly, Jr., C. N. Kimberlin, Jr., W. H. Miller, and H. V. Drushel, Coke Formation on Silica−Alumina Cracking Catalysts, *Ind. Eng. Chem. Proc. Des. Develop.* **5**, 193 (1966).

2. W. H. Miller, New Equation for Lower Bounds to Eigenvalues with Application to the Helium Atom, *J. Chem. Phys.* **42**, 4305 (1965).

3. W. H. Miller, On the Variation-Perturbation Method for Excited States, *J. Chem. Phys.* **44**, 2198 (1966).

4. W. H. Miller, Resonances in the Scattering of Electrons from Atoms, *Phys. Rev.* **152**, 70 (1966).

5. W. H. Miller, Extension of Gay's Equation for Lower Bounds to Eigenvalues, *J. Chem. Phys.* **48**, 530 (1968).

6. W. H. Miller, Uniform Semiclassical Approximations for Elastic Scattering and Eigenvalue Problems, *J. Chem. Phys.* **48**, 464 (1968).

7. W. H. Miller, Semiclassical Treatment of Multiple Turning-Point Problems Phase Shifts and Eigenvalues, *J. Chem. Phys.* **48**, 1651 (1968).

8. W. H. Miller, Distorted Wave Theory for Collisions of an Atom and a Diatomic Molecule, *J. Chem. Phys.* **49**, 2373 (1968).

9. W. H. Miller, Coupled Equations and the Minimum Principle for Collisions of an Atom and a Diatomic Molecule, Including Rearrangements, *J. Chem. Phys.* **50**, 407 (1969).

10. W. H. Miller, Final-State Interactions in Collisions of an Atom and a Diatomic Molecule, *J. Chem. Phys.* **50**, 931 (1969).

11. W. H. Miller, Improved Equation for Lower Bounds to Eigenvalues; Bounds for the Second-Order Perturbation Energy, *J. Chem. Phys.* **50**, 2758 (1969).

12. W. H. Miller, Semiclassical Approximation for the Total Cross Section of Atom−Diatomic Molecule Collisions; Quenching of Glory Undulations, *J. Chem. Phys.* **50**, 3124 (1969).

13. W. H. Miller, On the Possibility of Extracting Anistropy Parameters from the M-Dependence of Total Cross Section Measurements, *J. Chem. Phys.* **50**, 3410 (1969).

14. W. H. Miller, On the Possibility of Extracting Anisotropy Parameters from Total Cross Section Measurements. II, *J. Chem. Phys.* **50**, 3868 (1969).

15. W. H. Miller, WKB Solution of Inversion Problems for Potential Scattering, *J. Chem. Phys.* **51**, 3631 (1969).

16. W. H. Miller, Study of the Statistical Model for Molecular Collisions, *J. Chem. Phys.* **52**, 543 (1970).

17. W. H. Miller, Computation of Autoionization Lifetimes via a "Golden-Rule"-Like Formula, *Chem. Phys. Lett.* **4**, 627 (1970).

18. W. H. Miller, Theory of Penning Ionization, *J. Chem. Phys.* **52**, 3563 (1970).

19. W. H. Miller and H. F. Schaefer, Theoretical Treatment of Penning Ionization He(1s2s$^1$,$^3$S) + H, *J. Chem. Phys.* **53**, 1421 (1970).

20. W. H. Miller, Semiclassical Theory of Atom−Diatom Collisions: Path Integrals and the Classical S-Matrix, *J. Chem. Phys.* **53**, 1949 (1970).

21. W. H. Miller, The Classical S-Matrix: Numerical Application to Inelastic Collisions, *J. Chem. Phys.* **53**, 3578 (1970).

22. W. H. Miller, The Classical S-Matrix: A More Detailed Study of Classically Forbidden Transitions in Inelastic Collisions, *Chem. Phys. Lett.* **7**, 431 (1970).

23. W. H. Miller, The Semiclassical Nature of Atomic and Molecular Collisions, *Acc. Chem. Res.* **4**, 161 (1971).

24. W. H. Miller, Additional WKB Inversion Relations for Bound-State and Scattering Problems, *J. Chem. Phys.* **54**, 4174 (1971).

25. W. H. Miller, The Classical S-Matrix for Rotational Excitation; Quenching of Quantum Effects in Molecular Collisions, *J. Chem. Phys.* **54**, 5386 (1971).

26. C. A. Slocomb, W. H. Miller and H. F. Schaefer, Collisional Quenching of Metastable Hydrogen Atoms, *J. Chem. Phys.* **55**, 926 (1971).

27. W. H. Miller, Molecular Ramsauer-Townsend Effect in Very Low Energy He$^4$−He$^4$ Scattering, *Chem. Phys. Lett.* **10**, 7 (1971). Addendum **11**, 152 (1971).

28. W. H. Miller, Classical Path Approximation for the Boltzmann Density Matrix, *J. Chem. Phys.* **55**, 3146 (1971).

29. C. C. Rankin and W. H. Miller, Classical S-Matrix for Linear Reactive Collisions of H + Cl$_2$, *J. Chem. Phys.* **55**, 3150 (1971).

30. H. F. Schaefer and W. H. Miller, Curve Crossing of the B$^3\Sigma_u$- and $^3\Pi_v$ States and its Relation to Predissociation in the Schumann−Runge Bands, *J. Chem. Phys.* **55**, 4107 (1971).

31. W. H. Miller, Simple Error Bound for Coupled-Channel Scattering Calculations, *Chem. Phys. Lett.* **11**, 535 (1971).

32. W. H. Miller, Classical-Limit Green's Function (Fixed-Energy Propagator) and Classical Quantization of Non-Separable Systems, *J. Chem. Phys.* **56**, 38 (1972).

33. W. H. Miller, Classical Limit of Fredholm Theory for Elastic and Inelastic Scattering; Inability of Phase Space Integrals to Describe Inelastic Transitions, *J. Chem. Phys.* **56**, 745 (1972).

34. W. H. Miller, C. A. Slocomb, and H. F. Schaefer, Molecular Autoionization Lifetimes and Cross Sections for Penning Ionization: Numerical Results for He*-(1s2s$^3$S) + H(1s$^2$S), *J. Chem. Phys.* **56**, 1347 (1972).

35. S. M. Hornstein and W. H. Miller, Quantum Corrections (Within the Classical Path Approximation) to the Boltzmann Density Matrix, *Chem. Phys. Lett.* **13**, 298 (1972).

36. G. Wolken, W. H. Miller, and M. Karplus, Theoretical Studies of H + H$_2$ Rotationally Inelastic Scattering, *J. Chem. Phys.* **56**, 4930 (1972).

37. W. H. Miller and T. F. George, Semiclassical Theory of Electronic Transitions in Low Energy Atomic and Molecular Collisions Involving Several Nuclear Degrees of Freedom, *J. Chem. Phys.* **56**, 5637 (1972).

38. W. H. Miller and T. F. George, Analytic Continuation of Classical Mechanics for Classically Forbidden Collisions Processes, *J. Chem. Phys.* **56**, 5668 (1972).

39. T. F. George and W. H. Miller, Complex-Valued Classical Trajectories for Linear Reactive Collisions of H + H$_2$ Below the Classical Threshold, *J. Chem. Phys.* **56**, 5722 (1972).

40. T. F. George and W. H. Miller, Classical S-Matrix Theory of Reactive Tunneling: Linear H + H$_2$ Collisions, *J. Chem. Phys.* **57**, 2458 (1972).

41. T. F. George and W. H. Miller, Open-Channel Projectors for Rearrangement Processes in Molecular Collisions, *Phys. Rev. A*. **6**, 1885 (1972).

42. J. D. Doll and W. H. Miller, Classical-Limit Quantization of Non-Separable Systems: Multi-Dimensional WKB Perturbation Theory, *J. Chem. Phys.* **57**, 4428 (1972).

43. J. D. Doll and W. H. Miller, Classical S-Matrix for Vibrational Excitation of H$_2$ by Collision with He in Three Dimensions, *J. Chem. Phys.* **57**, 5019 (1972).

44. J. D. Doll, T. F. George, and W. H. Miller, Complex-Valued Classical Trajectories for Reactive Tunneling in Three-Dimensional Collisions of H and H$_2$, *J. Chem. Phys.* **58**, 1343 (1973).

45. W. H. Miller, Improved Classical Path Approximation for the Boltzmann Density Matrix, *J. Chem. Phys.* **58**, 1664 (1973).

46. S. A. Augustin, W. H. Miller, P. K. Pearson, and H. F. Schaefer, Potential Curves and Inelastic Cross Sections for Low Energy Collisions of O$^+$ and He, *J. Chem. Phys.* **58**, 2845 (1973).

47. T. F. George and W. H. Miller, Classically Forbidden Collision Processes, in *Energy, Structure and Reactivity*, ed. D. W. Smith and W. B. McRae, Wiley, p. 76, (1973).

48. B. J. Garrison, W. H. Miller and H. F. Schaefer, Penning and Associative Ionization of Triplet Metastable Helium Atoms, *J. Chem. Phys.* **59**, 3193 (1973).

49. W. H. Miller and A. W. Raczkowski, Partial Averaging in Classical S-Matrix Theory; Vibrational Excitation of H$_2$ by He, *Faraday Disk. Chem. Soc.* **55**, 45 (1973).

50. W. H. Miller, Semiclassical Methods in Reactive and Non-Reactive Collisions, in *The Physics of Electronic and Atomic Collisions*, eds. B. C. Cobic and M. V. Kurepa, Institute of Physics, Belgrade, p. 503 (1973).

51. W. H. Miller, Classical-Limit Quantum Mechanics and the Theory of Molecular Collisions, *Adv. Chem. Phys.* **25**, 69 (1974).

52. R. K. Preston, C. Sloane, and W. H. Miller, Semiclassical Theory of Collisionally Induced Fine-Structure Transitions in Fluorine Atoms, *J. Chem. Phys.* **60**, 4961 (1974).

53. S. M. Hornstein and W. H. Miller, Modified Classical S-Matrix for Tunneling in the Collinear H + H$_2$ Reaction, *J. Chem. Phys.* **61**, 745 (1974).

54. W. H. Miller, Quantum Mechanical Transition State Theory and a New Semiclassical Model for Reaction Rate Constants, *J. Chem. Phys.* **61**, 1823 (1974).

55. S. D. Augustin and W. H. Miller, Classical Trajectory Study of Rotational Excitation in Low Energy He−CO and He−H$_2$ Collisions, *Chem. Phys. Lett.* **28**, 149 (1974).

56. S. D. Augustin and W. H. Miller, Semiclassical Treatment of Atom-Asymmetric Rotor Collisions; Rotational Excitation of Formaldehyde at Low Energies, *J. Chem. Phys.* **61**, 3155 (1974).

57. A. W. Raczkowski and W. H. Miller, Classical S-Matrix Calculation for Vibrationally Inelastic Transitions in Three-Dimensional Collisions of Li$^+$ with H$_2$, *J. Chem. Phys.* **61**, 5413 (1974).

58. R. I. Masel, R. P. Merrill, and W. H. Miller, Semiclassical Trajectory Calculations of Helium Scattering from W(112), *Surf. Sci.* **46**, 681 (1974).

59. G. E. Zahr, R. K. Preston, and W. H. Miller, Theoretical Treatment of Quenching in O($^1$D) + N$_2$ Collisions, *J. Chem. Phys.* **62**, 1127 (1975).

60. S. Chapman, S. M. Hornstein, and W. H. Miller, Accuracy of Transition State Theory for the Threshold of Chemical Reactions with Activation Energy: Collinear and Three-Dimensional H + H$_2$, *J. Am. Chem. Soc.* **97**, 892 (1975).

61. W. H. Miller, Semiclassical Limit of Quantum Mechanical Transition State Theory for Non-Separable Systems, *J. Chem. Phys.* **62**, 1899 (1975).

62. W. H. Miller, The Classical S-Matrix in Molecular Collisions, *Adv. Chem. Phys.* **30**, 77 (1975).

63. W. H. Miller, Semiclassical Quantization of Non-Separable Systems: A New Look at Periodic Orbit Theory, *J. Chem. Phys.* **63**, 996 (1975).

64. W. H. Miller, Path Integral Representation of the Reaction Rate Constant in Quantum Mechanical Transition State Theory, *J. Chem. Phys.* **63**, 1166 (1975).

65. R. N. Porter, L. M. Raff, and W. H. Miller, Quasiclassical Selection of Initial Coordinates and Momenta for a Rotating Morse Oscillator, *J. Chem. Phys.* **63**, 2214 (1975).

66. G. E. Zahr and W. H. Miller, Semiclassical Theory of Diffraction in Elastic Scattering, *Mol. Phys.* **30**, 951 (1975).

67. S. Chapman, B. C. Garrett, and W. H. Miller, Semiclassical Transition State Theory for Non-Separable Systems: Application to the Collinear H + H$_2$ Reaction, *J. Chem. Phys.* **63**, 2710 (1975).

68. F. T. Smith, D. L. Huestis, D. Mukherjee, and W. H. Miller, Semiclassical Perturbation Scattering by a Rigid Dipole, *Phys. Rev. Lett.* **35**, 1073 (1975).

69. B. J. Garrison, W. A. Lester, W. H. Miller, and S. Green, Cooling of the 6 and 2 cm Doublets of Interstellar H$_2$-CO by Collision: An Accurate Quantum Mechanical Calculation, *Astrophys. J.* **200**, L175 (1975).

70. R. I. Masel, R. P. Merrill, and W. H. Miller, Quantum Scattering from a Sinusoidal Hard-Wall−Atomic Diffraction from Solid Surfaces, *Phys. Rev. B* **12**, 5545 (1975).

71. R. I. Masel, R. P. Merrill, and W. H. Miller, Semiclassical Model for Atomic Scattering from Solid Surfaces−He and Ne Scattering from W(112), *J. Chem. Phys.* **64**, 45 (1976).

72. A. P. Hickman, A. D. Isaacson, and W. H. Miller, Calculation of Autoionization States of He and H$^-$, *Chem. Phys. Lett.* **37**, 63 (1976).

73. S. Chapman, B. C. Garrett, and W. H. Miller, Semiclassical Eigenvalues for Non-Separable Systems: Non-Perturbative Solution of the Hamilton-Jacobi Equation in Action-Angle Variables, *J. Chem. Phys.* **64**, 502 (1976).

74. R. I. Masel, R. P. Merrill, and W. H. Miller, Semiclassical Theories and Quantum Hardwall Calculations of Atom−Surface Scattering, *J. Vac. Sci. Tech.* **13**, 355 (1976).

75. W. H. Miller, On the Existence of Semiclassical Eigenvalues for Irregular Spectra, *J. Chem. Phys.* **64**, 2880 (1976).

76. W. H. Miller, Importance of Non-Separability in Quantum Mechanical Transition State Theory, *Acc. Chem. Res.* **9**, 306 (1976).

77. B. J. Garrison, W. A. Lester, and W. H. Miller, Coupled Channel Study of Rotational Excitation of a Rigid Asymmetric Top by Atom Impact: (H$_2$CO, He) at Interstellar Temperatures, *J. Chem. Phys.* **65**, 2193 (1976).

78. W. H. Miller, Unified Statistical Theory for "Complex" and "Direct" Reaction Mechanisms, *J. Chem. Phys.* **65**, 2216 (1976).

79. R. I. Masel, R. P. Merrill, and W. H. Miller, Atomic Scattering from a Sinusoidal Hard Wall: Comparison of Approximate Methods with Exact Quantum Results, *J. Chem. Phys.* **65**, 2690 (1976).

80. W. H. Miller, Recent Developments in Semiclassical Mechanics: Eigenvalues and Reaction Rate Constants, *The New World of Quantum Chemistry*, ed. B. Pullman and R. Parr, D. Reidel Publishing Co., Dordrecht (Netherlands), 1976, pp. 87−102.

81. W. H. Miller, Editor, *Dynamics of Molecular Collisions*, Part A, Volume 1 of *Modern Theoretical Chemistry*, Plenum Press, N. Y., 1976.

82. W. H. Miller, Editor, *Dynamics of Molecular Collisions*, Part B, Volume 2 of *Modern Theoretical Chemistry*, Plenum Press, N. Y., 1976.

83. H. F. Schaefer and W. H. Miller, Large Scale Scientific Computation via Minicomputer, *Comp. Chem.* **1**, 85 (1976).

84. N. C. Handy, S. M. Colwell, and W. H. Miller, Semiclassical Methods for Vibrational Energy Levels of Triatomic Molecules, *Faraday Disk. Chem. Soc.* **62**, 29 (1977).

85. W. H. Miller, Semiclassical Theory for Non-Separable Systems: Construction of "Good" Action-Angle Variables for Reaction Rate Constants, *Faraday Disk. Chem. Soc.* **62**, 40 (1977).

86. A. P. Hickman, A. D. Isaacson, and W. H. Miller, Feshbach Projection Operator Calculation of the Potential Energy Surfaces and Autoionization Lifetimes for He($2^3$S)−H and He($2^3$S)−H$_2$, *J. Chem. Phys.* **66**, 1483, (1977).

87. A. P. Hickman, A. D. Isaacson, and W. H. Miller, Penning Ionization of H$_2$ by He($2^3$S): Quantum Mechanical Scattering Calculations within the Rigid-Rotor Approximation, *J. Chem. Phys.* **66**, 1492 (1977).

88. A. D. Isaacson, A. P. Hickman, and W. H. Miller, Penning Ionization of H$_2$ by He$^*$: Calculation of Anomalous Structure in the Singlet Interaction Potential, *J. Chem. Phys.* **67**, 370 (1977).

89. C. W. McCurdy and W. H. Miller, Interference Effects in Rotational State Distributions; Propensity and Inverse Propensity, *J. Chem. Phys.* **67**, 463 (1977).

90. W. H. Miller and H. Morgner, A Unified Treatment of Penning Ionization and Excitation Transfer, *J. Chem. Phys.* **67**, 4923 (1977).

91. J. E. Adams and W. H. Miller, Semiclassical Eigenvalues for Potential Functions Defined on a Finite Interval, *J. Chem. Phys.* **67**, 5775 (1977).

92. R. M. Stratt and W. H. Miller, A Phase Space Sampling Approach to Equilibrium Semiclassical Statistical Mechanics, *J. Chem. Phys.* **67**, 5894 (1977).

93. C. W. McCurdy and W. H. Miller, A New Helicity Representation for Reactive Atom−Diatom Collisions, in *State-to-State Chemistry*, eds. P. R. Brooks and E. F. Hayes, ACS Symp. Ser. **56**, 239 (1977).

94. P. K. Pearson, R. R. Lucchese, W. H. Miller, and H. F. Schaefer, Theoretical Chemistry via Minicomputer, in *Minicomputers and Large Scale Computations*, ed. P. Lykos, ACS Symp. Ser. **57**, 171 (1977).

95. W. H. Miller, Some Recent Developments in Statistical Theories of Chemical Reactions, in *Physicochemical Hydrodynamics* (V. G. Levich Festchrift), and ed. D. B. Spalding, Advanced Publications Ltd., London, 1977, pp. 845-856.

96. W. H. Miller and B. M. Skuse, On the Possibility of Direct Solution of the Classical Liouville for Inelastic Molecular Collisions; the Reduced Liouville Equation, *J. Chem. Phys.* **68**, 295 (1978).

97. S. M. Colwell, N. C. Handy, and W. H. Miller, A Semiclassical Determination of the Energy Levels of a Rigid Asymmetric Rotor, *J. Chem. Phys.* **68**, 745 (1978).

98. W. H. Miller and F. T. Smith, Semiclassical Perturbation Theory of Electron−Molecule Collisions, *Phys. Rev. A* **17**, 939 (1978).

99. S. Green, B. J. Garrison, W. A. Lester, and W. H. Miller, Collisional Excitation of Interstellar Formaldehyde, *Astrophys. J.* **222**, 1117 (1978): *Astrophys. J. Suppl. Ser.* **37**, 321 (1978).

100. B. C. Garrett and W. H. Miller, Quantum Mechanical Reactive Scattering via Exchange Kernels: Application to the Collinear H + H$_2$ Reaction, *J. Chem. Phys.* **68**, 4051 (1978).

101. W. H. Miller, Resonance Effects in the Semiclassical Theory of Electronically Non-Adiabatic Collision Processes, *J. Chem. Phys.* **68**, 4431 (1978).

102. W. H. Miller, A Classical/Semiclassical Theory for the Interaction of Infrared Radiation with Molecular Systems, *J. Chem. Phys.* **69**, 2188 (1978).

103. A. E. Orel and W. H. Miller, Infrared Laser Induced Chemical Reactions, *Chem. Phys. Lett.* **57**, 362 (1978).

104. A. W. Raczkowski, W. A. Lester, Jr., and W. H. Miller, Vibrational Relaxation in the para-H$_2$-$^4$He System: Comparison of Coupled-Channel, Coupled-States, and Effective Potential Methods, *J. Chem. Phys.* **69**, 2692 (1978).

105. A. D. Isaacson, C. W. McCurdy, and W. H. Miller, On the Possibility of Calculating Siegert Eigenvalues for Autoionizing Electronic States, *Chem. Phys.* **34**, 311 (1978).

106. W. H. Miller and C. W. McCurdy, Classical Trajectory Model for Electronically Non-Adiabatic Collision Phenomena: A Classical Model for Electronic Degrees of Freedom, *J. Chem. Phys.* **69**, 5163 (1978).

107. S. M. Colwell, N. C. Handy and W. H. Miller, Semiclassical Eigenvalues for Rotating Triatomic Molecules, in *Stochastic Behavior in Classical and Quantum Hamiltonian Systems*, eds. G. Casati and J. Ford, Springer Verlag, N. Y., 1978, p. 299.

108. A. D. Isaacson and W. H. Miller, Calculation of Siegert Eigenvalues for Molecular Systems: Results for He-($2^{1,3}$S) + H$_2$, *Chem. Phys. Lett.* **62**, 374 (1979).

109. A. E. Orel and W. H. Miller, Infrared Laser Enhancement of Chemical Reactions via Collision Induced Absorption, *J. Chem. Phys.* **70**, 4393, (1979).

110. J. E. Adams and W. H. Miller, On Expansion of Exchange Kernels for Reactive Scattering, *J. Phys. Chem.* **83**, 1505 (1979).

111. C. W. McCurdy, H. D. Meyer, and W. H. Miller, Classical Model for Electronic Degrees of Freedom in Non-Adiabatic Collision Processes: Pseudo-Potential Analysis and Calculations for $F(^2P_{1/2}) + H^+$, $Xe \rightarrow F(^2P_{3/2}) + H^+$, Xe, *J. Chem. Phys.* **70**, 3177 (1979).

112. H. D. Meyer and W. H. Miller, A Classical Analogue for Electronic Degrees of Freedom in Non-Adiabatic Collision Processes, *J. Chem. Phys.* **70**, 3214 (1979).

113. A. D. Bandrauk and W. H. Miller, Analysis of the Generalized Stueckelberg Method of Non-Adiabatic Transitions, *Mol. Phys.* **38**, 1893 (1979).

114. W. H. Miller, On the Periodic Orbit Description of Tunneling in Symmetric and Asymmetric Double-Well Potential, *J. Phys. Chem.* **83**, 960 (1979).

115. J. E. Adams and W. H. Miller, A Unified Model for Diffractive and Inelastic Scattering of a Light Atom from a Solid Surface, *Surf. Sci.* **85**, 77 (1979).

116. W. H. Miller, Tunneling Corrections to Unimolecular Rate Constants, with Application to Formaldehyde, *J. Am. Chem. Soc.* **101**, 6810 (1979).

117. A. E. Orel and W. H. Miller, Infrared Laser Induced Chemical Reactions; Calculations for $X + H_2 \rightarrow HX + H$, in *Rarefied Gas Dynamics*, ed. R. Campargue, Comissariat a L′Energie Atomique, Paris, 1979, p. 1061.

118. H. D. Meyer and W. H. Miller, Classical Models for Electronic Degrees of Freedom: Derivation via Spin Analogy and Application to $F^* + H_2 \rightarrow F + H_2$, *J. Chem. Phys.* **71**, 2156 (1979).

119. R. M. Stratt, N. C. Handy, and W. H. Miller, On the Quantum Mechanical Implications of Classical Ergodicity, *J. Chem. Phys.* **71**, 3311 (1979).

120. W. H. Miller, N. C. Handy and J. E. Adams, Reaction Path Hamiltonian for Polyatomic Molecules, *J. Chem. Phys.* **72**, 99 (1980).

121. W. H. Miller, Reply to a Comment by Milonni on "A Classical Semiclassical Theory for the Interaction of Infrared Radiation with Molecular Systems", *J. Chem. Phys.* **72**, 788 (1980).

122. H. D. Meyer and W. H. Miller, Analysis and Extension of Some Recently Proposed Classical Models for Electronic Degrees of Freedom, *J. Chem. Phys.* **72**, 2272 (1980).

123. A. E. Orel and W. H. Miller, Collision Induced Absorption Spectra for Gas-Phase Chemical Reaction in a High Power IR Laser Field, *J. Chem. Phys.* **72**, 5139 (1980).

124. A. E. Orel and W. H. Miller, Classical Model for Laser-Induced Non-Adiabatic Collision Processes, *J. Chem. Phys.* **73**, 241 (1980).

125. S. K. Gray, W. H. Miller, Y. Yamaguchi, and H. F. Schaefer, Reaction Path Hamiltonian: Tunneling Effects in the Unimolecular Isomerization HNC $\rightarrow$ HCN, *J. Chem. Phys.* **73**, 2733 (1980).

126. C. W. McCurdy and W. H. Miller, Progress in the Application of Classical S-Matrix Theory to Inelastic Collision Processes, *J. Chem. Phys.* **73**, 3191 (1980).

127. B. A. Waite and W. H. Miller, Model Studies of Mode-Specificity in Unimolecular Reaction Dynamics, *J. Chem. Phys.* **73**, 3713 (1980).

128. A. E. Orel and W. H. Miller, Enhancement of Chemical Reactions by Collision Induced Absorption of Infrared Laser Radiation, in *Electronic and Atomic Collisions*, eds. N. Oda and K. Takayanagi, 1980, North-Holland Pub., pp. 719.

129. W. H. Miller, Reaction Path Hamiltonian for Polyatomic Systems: Further Developments and Applications, in *Potential Energy Surfaces and Dynamical Calculations*, ed. D. G. Truhlar, Plenum Press, N. Y., 1981, p. 265.

130. S. K. Gray, W. H. Miller, Y. Yamaguchi, and H. F. Schaefer, Tunneling in the Unimolecular Decomposition of Formaldehyde, A More Quantitative Study, *J. Am. Chem. Soc.* **103**, 1900 (1981).

131. Y. Osamura, H. F. Schaefer, S. K. Gray, and W. H. Miller, Vinylidene, A Shallow Minimum on the $C_2H_2$ Potential Energy Surface: Static and Dynamical Considerations, *J. Am. Chem. Soc.* **103**, 1904 (1981).

132. B. A. Waite and W. H. Miller, Mode-Specificity in Unimolecular Reaction Dynamics: The Henon-Heiles Potential Energy Surface, *J. Chem. Phys.* **74**, 3910 (1981).

133. A. E. Orel, D. P. Ali and W. H. Miller, Classical Model for Electronically Non-Adiabatic Collision Processes: Resonance Effects in Electronic-Vibrational Energy Transfer, *Chem. Phys. Lett.* **79**, 137 (1981).

134. W. H. Miller and A. E. Orel, Classical Trajectory Models for Electronically Non-Adiabatic Collision Processes: A Classical Valence Bond Model for Electronic Degrees of Freedom, *J. Chem. Phys.* **74**, 6075 (1981).

135. W. H. Miller and S−H. Shi, Unified Semiclassical Perturbation and Infinite Order Sudden Approximation, With Application to the Reaction Path Hamiltonian Model, *J. Chem. Phys.* **75**, 2258 (1981).

136. C. J. Cerjan and W. H. Miller, On Finding Transition States, *J. Chem. Phys.* **75**, 2800 (1981).

137. C. J. Cerjan, S−H. Shi, and W. H. Miller, Applications of a Simple Dynamical Model to the Reaction Path Hamiltonian: Tunneling Corrections to Rate Constants, Product State Distributions, Line Widths of Local Mode Overtones, and Mode-Specificity in Unimolecular Decomposition, *J. Phys. Chem.* **86**, 2244 (1982).

138. B. A. Waite and W. H. Miller, A Semiclassical Multi-channel Branching Model for Describing State-Specific Unimolecular Decomposition and Other Dynamical Processes in Polyatomic Molecular Systems, *J. Chem. Phys.* **76**, 2412 (1982).

139. W. H. Miller, Effect of Reaction Path Curvature and Dimensionality on the Accuracy of Classical Transition State Theory, *J. Chem. Phys.* **76**, 4904 (1982).

140. W. H. Miller, Chemical Dynamics, *McGraw-Hill Encyclopedia of Science and Technology*, fifth Edition, McGraw-Hill, 1982, p. 50.

141. W. H. Miller and S. Schwartz, System-Bath Decomposition of the Reaction Path Hamiltonian for Polyatomic Scattering; Quantum Perturbative Treatment, *J. Chem. Phys.* **77**, 2378 (1982).

142. S. K. Gray and W. H. Miller, Classical Model for Electronic Degrees of Freedom: Charge Transfer in Na + I Collisions, *Chem. Phys. Lett.* **93**, 341 (1982).

143. C. Hiller, J. Manz, W. H. Miller and J. Römelt, Oscillating Reactivity of Collinear Symmetric Heavy + Light-Heavy Reactions, *J. Chem. Phys.* **78**, 3850 (1983).

144. W. H. Miller, Dynamical Effects of Symmetry along a Reaction Path; Mode Specificity in the Unimolecular Dissociation of Formaldehyde, *J. Am. Chem. Soc.* **105**, 216 (1983).

145. B. A. Waite, S. K. Gray and W. H. Miller, Mode Specificity in the Unimolecular Dissociation of Formaldehyde ($H_2CO \rightarrow H_2 + CO$), a Two-Mode Model, *J. Chem. Phys.* **78**, 259 (1983).

146. L. M. Hubbard and W. H. Miller, Application of the Semiclassical Perturbation (SCP) Approximation to Diffraction and Rotationally Inelastic Scattering of Atoms and Molecules from Surfaces, *J. Chem. Phys.* **78**, 1801 (1983).

147. J. Bicerano, H. F. Schaefer, and W. H. Miller, Structure and Tunneling Dynamics of Malonaldehyde, a Theoretical Study, *J. Am. Chem. Soc.* **105**, 2550 (1983).

148. W. H. Miller, Symmetry-Adapted Transition State Theory and a Unified Treatment of Multiple Transition States, *J. Phys. Chem.* **87**, 21 (1983).

149. L. M. Hubbard, S−H. Shi, and W. H. Miller, Multi-Channel Distorted Wave Born Approximation for Reactive Scattering, *J. Chem. Phys.* **78**, 2381 (1983).

150. D. P. Ali and W. H. Miller, Effect of Electronic Transition Dynamics on Iodine Atom Recombination in Liquids, *J. Chem. Phys.* **78**, 6640 (1983).

151. S. Schwartz and W. H. Miller, System-Bath Decomposition of the Reaction Path Hamiltonian. II. Rotationally Inelastic Reactive Scattering of $H + H_2$ in Three Dimensions, *J. Chem. Phys.* **79**, 3759 (1983).

152. W. H. Miller, Symmetry Adapted Transition State Theory: Non-Zero Total Angular Momentum, *J. Phys. Chem.* **87**, 2731 (1983).

153. W. H. Miller, On the Question of Mode-Specificity in Unimolecular Reaction Dynamics, *Laser Chem.* **2**, 243 (1983).

154. W. H. Miller, Reaction Path Dynamics for Polyatomic Systems, *J. Phys. Chem.* **87**, 3811 (1983).

155. W. H. Miller, S. D. Schwartz, and J. W. Tromp, Quantum Mechanical Rate Constants for Bimolecular Reactions, *J. Chem. Phys.* **79**, 4889 (1983).

156. D. P. Ali and W. H. Miller, Classical Models for Electronic Degrees of Freedom: Quenching of $Br^*(^2P_{1/2})$ by Collision with $H_2$ in Three Dimensions, *Chem. Phys. Lett.* **103**, 470 (1984).

157. T. Carrington, Jr., L. M. Hubbard, H. F. Schaefer, and W. H. Miller, Vinylidene: Potential Energy Surface and Unimolecular Reaction Dynamics, *J. Chem. Phys.* **80**, 4347 (1984).

158. L. M. Hubbard and W. H. Miller, Application of the Semiclassical Perturbation Approximation to Scattering from Surfaces: Generalization to Include Phonon Inelasticity, *J. Chem. Phys.* **80**, 5827 (1984).

159. D. P. Ali and W. H. Miller, Geminate Recombination of Iodine Atoms in Solution: a Generalized Langevin Treatment Including the Effect of Electronically Inelastic Transitions, *Chem. Phys. Lett.* **105**, 501 (1984).

160. G. C. Schatz, L. M. Hubbard, P. S. Dardi, and W. H. Miller, Coupled Channel Distorted Wave Calculations for the Three-Dimensional $H + H_2$ Reaction, *J. Chem. Phys.* **81**, 231 (1984).

161. W. H. Miller, Calculation of Semiclassical Eigenvalues with One Arbitrary Trajectory, *J. Chem. Phys.* **81**, 3573 (1984).

162. E. Pollak and W. H. Miller, A New Physical Interpretation for Time in Scattering Theory, Phys. Rev. Lett. **53**, 115 (1984).

163. T. Carrington, Jr. and W. H. Miller, Reaction Surface Hamiltonian for the Dynamics of Reactions in Polyatomic Systems, *J. Chem. Phys.* **81**, 3942 (1984).

164. R. Jaquet and W. H. Miller, Quantum Mechanical Rate Constants via Path Integrals: Diffusion of Hydrogen Atoms on a W(100) Surface, *J. Phys. Chem.* **89**, 2139 (1985).

165. M. J. Frisch, B. Liu, J. S. Binkley, H. F. Schaefer, and W. H. Miller, Further Theoretical Examination of the F $+ H_2$ Entrance Channel Barrier, *Chem. Phys. Lett.* **114**, 1 (1985).

166. S−H. Shi and W. H. Miller, A Semiclassical Model for Intramolecular Vibrational Relaxation of Local Mode Overtone States in Polyatomic Molecules, *Theor. Chim. Acta* **68**, 1 (1985).

167. P. S. Dardi, S−H. Shi, and W. H. Miller, Quantum Mechanical Reactive Scattering via Exchange Kernels: Infinite Order Exchange on a Grid, *J. Chem. Phys.* **83**, 575 (1985).

168. K. Yamashita and W. H. Miller, "Direct" Calculation of Quantum Mechanical Rate Constants via Path Integral Methods: Application to the Reaction Path Hamiltonian with Numerical Test for the $H + H_2$ Reaction in 3-D, *J. Chem. Phys.* **82**, 5475 (1985).

169. W. H. Miller, Semiclassical Methods in Chemical Dynamics, in *Semiclassical Descriptions of Atomic and Nuclear Collisions* (Niels Bohr Centennial Conferences), ed. J. Bang and J. deBoer, North Holland, 1985, pp. 9−28.

170. W. H. Miller, Some Recent Initiatives in Quantum Mechanical Reactive Scattering, in *Molecular Reaction Dynamics*, eds. R. Vetter and J. Vigue, Editions du Centre National de la Recherche Scientifique, Paris, 1986, pp. 147−162.

171. W. H. Miller, Reaction Path Models for Polyatomic Reaction Dynamics − from Transition State Theory to Path Integrals, in *The Theory of Chemical Reaction Dynamics*, ed. D. C. Clary, Reidel, Boston, 1986, pp. 27−45.

172. T. Carrington, Jr. and W. H. Miller, Reaction Surface Description of Intramolecular Hydrogen Atom Transfer in Malonaldehyde, *J. Chem. Phys.* **84**, 4364 (1986).

173. W. H. Miller and K. A. White, Classical Models for Electronic Degrees of Freedom: the Second-Quantized Many-Electron Hamiltonian, *J. Chem. Phys.* **84**, 5059 (1986).

174. N. C. Handy, T. J. Lee, and W. H. Miller, Spin−Orbit and Diagonal Born−Oppenheimer Corrections for the Reaction $F + H_2 \rightarrow HF + H$, *Chem. Phys. Lett.* **125**, 12 (1986).

175. W. H. Miller, Semiclassical Methods in Chemical Physics, *Science* **233**, 171 (1986).

176. J. W. Tromp and W. H. Miller, New Approach to Quantum Mechanical Transition State Theory, *J. Phys. Chem.* **90**, 3482 (1986).

177. W. H. Miller, Comment on "Probability Oscillations in Single Pass Curve Crossings: Semiclassical Predictions of Non-Monotonic Dependence on Crossing Velocity", *J. Chem. Phys.* **85**, 3703 (1986).

178. M. R. Hermann and W. H. Miller, Quantum Mechanical Reactive Scattering via Exchange Kernels: Comparison of Grid versus Basis Set Expansion of the Exchange Kernel, *Chem. Phys.* **109**, 163 (1986).

179. W. H. Miller, Reaction Paths and Surfaces for Hydrogen Atom Transfer Reactions in Polyatomic Molecules, in *Tunneling*, eds. J. Jortner and B. Pullman, D. Reidel, Boston, 1986, pp. 91−101.

180. W. H. Miller, Tunneling and State-Specificity in Unimolecular Reactions, *Chem. Rev.* **87**, 19 (1987).

181. N. Makri and W. H. Miller, Basis Set Methods for Describing the Quantum Mechanics of a ′System′ Interacting with a Harmonic "Bath", *J. Chem. Phys.* **86**, 1451 (1987).

182. W. H. Miller, A Schrödinger Equation Analogue to the Generalized Langevin Equation of Classical Mechanics, with Application to Reactive Flux Correlation Functions, in *Stochasticity and Intramolecular Redistribution of Energy*, eds. R. Lefebvre and S. Mukamel, D. Reidel, Boston, 1987, pp. 263−272.

183. W. H. Miller and B. M. D. D. Jansen op de Haar, A New Basis Set Method for Quantum Scattering Calculations, *J. Chem. Phys.* **86**, 6213 (1987).

184. J. Chang and W. H. Miller, Monte Carlo Path Integration in Real Time via Complex Coordinates, *J. Chem. Phys.* **87**, 1648 (1987).

185. W. H. Miller, Reactive Flux Correlation Functions and Monte Carlo Evaluation of Real Time Path Integrals, in *Few-Body Systems and Multiparticle Dynamics*, ed. D. A. Micha, Am. Inst. Physics, N. Y., 1987, pp. 245−260.

186. Y−T. Chang, Y. Yamaguchi, W. H. Miller, and H. F. Schaefer, An Analysis of the Infrared and Raman Spectra of the Formic Acid Dimer (HCOOH)$_2$, *J. Am. Chem. Soc.* **109**, 7245 (1987).

187. J. W. Tromp and W. H. Miller, The Reactive Flux Correlation Function for Collinear Reactions: H + H$_2$, Cl + HCl, F + H$_2$, *Faraday Disk. Chem. Soc.* **84**, 441 (1987).

188. N. Makri and W. H. Miller, Monte Carlo Integration with Oscillatory Integrands, with Implications for Feynman Path Integration in Real Time, *Chem. Phys. Lett.* **139**, 10 (1987).

189. N. Makri and W. H. Miller, Time-Dependent Self-Consistent Field (TDSCF) Approximation for a Reaction Coordinate Coupled to a Harmonic Bath:Single and Multi-Configuration Treatments, *J. Chem. Phys.* **87**, 5781 (1987).

190. J. Z. H. Zhang and W. H. Miller, New Method for Quantum Reactive Scattering, with Applications to the 3-D H + H$_2$ Reaction, *Chem. Phys. Lett.* **140**, 329 (1987).

191. B. A. Ruf and W. H. Miller, A New (Cartesian) Model for Reaction Dynamics in Polyatomic Systems, with Application to H−Atom Transfer in Malonaldehyde, *J. Chem. Soc., Faraday Trans. 2* **84**, 1523 (1988).

192. W. H. Miller, A New Variational Expression for the Scattering Matrix, *Collect. Czech. Chem. Comm.* **53**, 1873 (1988).

193. J. Z. H. Zhang, S. I. Chu, and W. H. Miller, Quantum Scattering via the S-Matrix Version of the Kohn Variational Principle, *J. Chem. Phys.* **88**, 6233 (1988).

194. W. F. Polik, C. B. Moore, and W. H. Miller, Quantum Interference Among Competing Unimolecular Decay Channels: Asymmetric D$_2$CO Decay Profiles, *J. Chem. Phys.* **89**, 3584 (1988).

195. J. Z. H. Zhang and W. H. Miller, Accurate 3-Dimensional Quantum Scattering Calculations for F + H$_2$ → HF + H, *J. Chem. Phys.* **88**, 4549 (1988).

196. N. Makri and W. H. Miller, Monte Carlo Path Integration for the Real Time Propagator, *J. Chem. Phys.* **89**, 2170 (1988).

197. J. Z. H. Zhang and W. H. Miller, Comment on "Quantum Scattering via the S-Matrix Version of the Kohn Variational Principle", *J. Chem. Phys.* **89**, 4454 (1988).

198. W. H. Miller, Effect of Fluctuations in State-Specific Unimolecular Rate Constants on the Pressure Dependence of the Average Unimolecular Reaction Rate, *J. Phys. Chem.* **92**, 4261 (1988).

199. W. H. Miller, Recent Developments in Quantum Mechanical Reactive Scattering-the S-Matrix Version of the Kohn Variational Principle, Comments At. *Mol. Phys.* **22**, 115 (1988).

200. W. H. Miller, Theoretical Models for Reaction Dynamics in Polyatomic Molecular Systems, in *New Theoretical Concepts for Understanding Organic Reactions*, eds. J. Bertran and I. G. Csizmadia, NATO ASI Series, Vol. 267, 1989, pp. 347−372.

201. W. H. Miller, B. A. Ruf, and Y. T. Chang, A Diabatic Reaction Path Hamiltonian, *J. Chem. Phys.* **89**, 6298 (1988).

202. N. Makri and W. H. Miller, Correct Short-Time Propagator for Feynman Path Integration by Power Series Expansion in $\Delta t$, *Chem. Phys. Lett.* **151**, 1 (1988).

203. A. C. Peet and W. H. Miller, A Pointwise Representation of the S-Matrix Kohn Variational Principle for Quantum Scattering, *Chem. Phys. Lett.* **149**, 257 (1988).

204. J. Z. H. Zhang and W. H. Miller, Quantum Reactive Scattering via the S-Matrix Version of the Kohn Variational Principle: Integral Cross Sections for H + H$_2$(v$_1$=j$_1$=0) → H$_2$(v$_2$=1,j$_2$=1,3) + H in the Energy Range E$_{total}$ = 0.9 eV − 1.4 eV, *Chem. Phys. Lett.* **153**, 465 (1988).

205. N. Makri and W. H. Miller, Exponential Power Series Expansion for the Quantum Time Evolution Operator, *J. Chem. Phys.* **90**, 904 (1989).

206. W. H. Miller, Quantum Mechanics of Chemical Reactions: Recent Developments in Reactive Scattering and in Reaction Path Hamiltonians, in *Perspectives in Quantum Chemistry,* eds. B. Pullman and J. Jortner, (Sixth Int. Cong. on Quant. Chem., Jerusalem)D. Reidel, pp. 57−82, (1989).

207. J. Z. H. Zhang and W. H. Miller, Reply to Comment on: Accurate Three-Dimensional Quantum Scattering Calculations for F + H$_2$ → HF + H, *J. Chem. Phys.* **90**, 7610 (1989).

208. J. Z. H. Zhang and W. H. Miller, Quantum Reactive Scattering via the S-Matrix Version of the Kohn Variational Principle: Differential and Integral Cross Sections for D + H$_2$ → HD + H, *J. Chem. Phys.* **91**, 1528 (1989).

209. J. Z. H. Zhang and W. H. Miller, Differential Cross Section (Angular Distribution) for the Reaction H + H$_2$(v=j=0) → H$_2$(v′, odd j′) + H in the Energy Range 0.90−1.35 eV, *Chem. Phys. Lett.* **159**, 130 (1989).

210. N. Makri and W. H. Miller, A Semiclassical Tunneling Model for Use in Classical Trajectory Simulations, *J. Chem. Phys.* **91**, 4026 (1989).

211. L. F. X. Gaucher and W. H. Miller, On the Absence of Anomalous Singularities in the S-Matrix Version of the Kohn Variational Principle of Quantum Scattering, *Isr. J. Chem.* **29**, 349 (1989).

212. G. A. Voth, D. Chandler, and W. H. Miller, Time Correlation Function and Path Integral Analysis of Quantum Constants, *J. Phys. Chem.* **93**, 7009 (1989).

213. W. H. Miller, W. L. Hase, and C. L. Darling, A Simple Model for Correcting the Zero Point Energy Problem in Classical Trajectory Simulations of Polyatomic Molecules, *J. Chem. Phys.* **91**, 2863 (1989).

214. W. Yang and W. H. Miller, Block Lanczos Approach Combined with Matrix Continued Fraction for the S-Matrix Kohn Variational Principle in Quantum Scattering, *J. Chem. Phys.* **91**, 3504 (1989).

215. W. Yang, A. C. Peet, and W. H. Miller, A Collocation Approach for Quantum Scattering Based on the S-Matrix Kohn Variational Principle, *J. Chem. Phys.* **91**, 7537 (1989).

216. G. A. Voth, D. Chandler, and W. H. Miller, Rigorous Formulation of Quantum Transition State Theory and its Dynamical Corrections, *J. Chem. Phys.* **91**, 7749 (1989).

217. W. H. Miller, Y.-T. Chang, and N. Makri, Some New Theoretical Methods for Treating Reaction Dynamics in Polyatomic Molecular Systems, in *Computational Advances in Organic Chemistry: Molecular Structure and Reactivity*, eds. C. Ögretir and I. G. Csizmadia, Kluwer, 1991, pp. 289−302.

218. Z. J. H. Zhang and W. H. Miller, Photodissociation and Continuum Resonance Raman Cross Sections, and General Franck−Condon Intensities, from S-Matrix Kohn Scattering Calculations, with Application to the Photoelectron Spectrum of $H_2F^- + h\nu \rightarrow H_2 + F$, HF $+ H + e^-$, *J. Chem. Phys.* **92**, 1811 (1990).

219. G. A. Voth, D. Chandler, and W. H. Miller, A New Perspective on Quantum Mechanical Transition State Theory, in *Quantum Simulations of Condensed Matter Phenomena*, eds. J. J. D. Dolland and J. E. Gubernatis, World Scientific Press, 1990, pp. 391−400.

220. W. F. Polik, D. R. Guyer, W. H. Miller, and C. B. Moore, Eigenstate-resolved Unimolecular Reaction Dynamics: Ergodic Character of $S_o$ Formaldehyde at the Dissociation Threshold, *J. Chem. Phys.* **92**, 3471 (1990).

221. Z. J. H. Zhang and W. H. Miller, Quasi-Adiabatic Basis Functions for the S-Matrix Kohn Variational Approach to Quantum Reactive Scattering, *J. Phys. Chem.* **94**, 7785 (1990).

222. S. M. Auerbach, J. Z. H. Zhang, and W. H. Miller, Comparison of Quantum Scattering Calculations for the $H + H_2$ Reaction using the LSTH and DMBE Potentials, *J. Chem. Soc. Faraday Trans.* **86**, 1701 (1990)

223. M. Moreno and W. H. Miller, On the Tautomerizatium Reaction 2-Pyridone ↔ 2-Hydroxypyridine: An Ab Initio Study, *Chem. Phys. Lett.* **171**, 475 (1990).

224. W. H. Miller, Quantum Mechanical Reactive Scattering Theory for Simple Chemical Reactions: Recent Developments in Methodology and Applications, AIP Conference Proceedings 205, *The Physics of Electronic and Atomic Collisions*, 1990, pp. 442−450.

225. Y.-T. Chang and W. H. Miller, An Empirical Valence Bond Model for Constructing Global Potential Energy Surfaces for Chemical Reactions of Polyatomic Molecular Systems, *J. Phys. Chem.* **94**, 5884 (1990).

226. W. H. Miller, Recent Advances in Quantum Mechanical Reactive Scattering Theory, Including Comparison of Recent Experiments with Rigorous Calculations of State-to-State Cross Section for the $H/D + H_2 \rightarrow H_2/HD +$ H Reaction, *Ann. Rev. Phys. Chem.* **41**, 245 (1990).

227. R. E. Continetti, J. Z. H. Zhang, and W. H. Miller, Comment on: Resonance Structure in the Energy-Dependence of State-to-State Differential Scattering Cross Section for the $D + H_2(v,j) \rightarrow HD(v',j') + H$ Reaction, *J. Chem. Phys.* **93**, 5356 (1990).

228. W. H. Miller, R. Hernandez, N. C. Handy, D. Jayatilaka, and A. Willetts, Ab Initio Calculation of Anharmonic Constants for a Transition State, with Application to Semiclassical Transition State Tunneling Probabilities, *Chem. Phys. Lett.* **172**, 62 (1990).

229. W. H. Miller, R. Hernandez, C. B. Moore, and W. F. Polik, A Transition State Theory-Based Statistical Distribution of Unimolecular Decay Rates, with Application to Unimolecular Decomposition of Formaldehyde, *J. Chem. Phys.* **93**, 5657 (1990).

230. J. Z. H. Zhang, D. L. Yeager and W. H. Miller, 3D Quantum Reactive Scattering Calculations of the Reaction $He + H_2+ \rightarrow HeH^+ + H$ for Total Angular Momentum $J = 0$, *Chem. Phys. Lett.* **173**, 489 (1990).

231. C. B. Moore, Q.-K. Zheng, Y. S. Choi, W. H. Green, S. K. Kim, A. J. Mahoney, W. H. Miller, C. D. Pibel, W. F. Polik and P. Teal, The High-Resolution Spectrosopy of Dissociating Molecules, *Phil. Trans. Roy. Soc. Lond. Ser. A* **332**, 297 (1990).

232. W. H. Miller and J. Z. H. Zhang, How to Observe the Elusive Resonances in H or $D + H_2 \rightarrow H_2$ or HD + H Reactive Scattering, *J. Phys. Chem.* **95**, 12 (1991).

233. W. H. Miller, Some New Approaches to Semiclassical and Quantum Transition StateTheory, *Ber. Bunsen-Ges Phys. Chem.* **95**, 389 (1991).

234. D. L. Yeager and W. H. Miller, Complex Log-Derivative Method for Non-Reactive Coupled-Channel Scattering Calculations, *J. Phys. Chem.* **95**, 8212 (1991).

235. W. H. Miller and T. Seideman, Transition State Theory, Siegert Eigenstates, and Quantum Mechanical Reaction Rates, *J. Chem. Phys.* **95**, 1768 (1991).

236. W. H. Miller, Comment on: Semiclassical Time Evolution without Root Searches, *J. Chem. Phys.* **95**, 9428 (1991).

237. T. Uzer and W. H. Miller, Theories of Intramolocular Vibrational Energy Transfer, *Phys. Rep.* **199**, 73 (1991).

238. J. Z. H. Zhang, W. H. Miller, A. Weaver, and D. Neumark, Quantum Reactive Scattering Calculations of Franck−Condon Factors for the Phtodetachment of $H_2F^-$ and $D_2F^-$ and Comparisons with Experiment, *Chem. Phys. Lett.* **182**, 283 (1991).

239. R. A. Harris, C. J. Grayce, N. Makri, and W. H. Miller, Comment on: A Corrected Exponential Power Series Expansion of the Position Matrix Elements of the Time Evolution Operator for a System in the Presence of a Vector Potential, *J. Chem. Phys.* **94**, 4682 (1991).

240. W. H. Miller, Quantum Mechanical Scattering for Chemical Reactions, in *Methods in Computational Molecular Physics*, ed. S. Wilson and G. H. F. Diercksen, Plenum, N. Y. 1992, pp. 519−533.

241. Y. T. Chang, C. Minichino, and W. H. Miller, Classical Trajectory Studies of the Molecular Dissociation Dynamics of Formaldehyde: $H_2CO \rightarrow H_2 + CO$, *J. Chem. Phys.* **96**, 4341 (1992).

242. W. H. Miller, Reaction Dynamics in Polyatomic Molecular Systems: Some Approaches for Constructing Potential Energy Surfaces and Incorporating Quantum Effects in Classical Trajectory Simulations, in *Molecular Aspects of Biotechnology: Computational Models and Theories*, ed. J. Bertran, Kluwer Academic Pub., pp. 193−235 (1992).

243. D. T. Colbert and W. H. Miller, A Novel Discrete Variable Representation (DVR) for Quantum Mechanical Reactive Scattering via the S-Matrix Kohn Method, *J. Chem. Phys.* **96**, 1982 (1992).

244. T. Seideman and W. H. Miller, Calculation of the Cumulative Reaction Probability via a Discrete Variable Representation with Absorbing Boundary Conditions, *J. Chem. Phys.* **96**, 4412 (1992).

245. M. J. Cohen, N. C. Handy, R. Hernandez, and W. H. Miller, Cumulative Reaction Probabilities for $H+H_2 \rightarrow H_2+H$ from a Knowledge of the Anharmonic Force Field, *Chem. Phys. Lett.* **192**, 407 (1992).

246. T. D. Sewell, D. L. Thompson, D. Gezelter, and W. H. Miller, Some Problems of Correcting the Zero-Point Energy Problem in Classical Trajectories, *Chem. Phys. Lett.* **193**, 512 (1992).

247. T. Seideman and W. H. Miller, Quantum Mechanical Reaction Probabilities via a Discrete Variable Representation-Absorbing Boundary Condition Green's Function, *J. Chem. Phys.* **97**, 2499 (1992).

248. W. H. Miller and T. Seideman, Cumulative and State-to-State Reaction Probabilities via a Discrete Variable Representation−Absorbing Boundary Condition Green's Function, in *Time Dependent Quantum Molecular Dynamics: Experiments and Theory*, ed. J. Broeckhove and L. Lathouwers, Plenum, N. Y., 1992, pp. 267−277.

249. G. Stock and W. H. Miller, A Classical Model for Time- and Frequency-Resolved Spectroscopy of Nonadiabatic Excited-State Dynamics, *Chem. Phys. Lett.* **197**, 396 (1992).

250. W. H. Miller, Beyond Transition State Theory ? A Rigorous Quantum Theory of Chemical Reaction Rates, *Acc. Chem. Res.* **26**, 174 (1993).

251. W. H. Miller, S-Matrix Version of the Kohn Variational Principle for Quantum Scattering Theory of Chemical Reactions, in *Advances in Molecular Vibrations and Collision Dynamics: Quantum Reactive Scattering*, Vol. IIA, ed. J. M. Bowman, JAI Press, Greenwich, 1994, pp. 1−32.

252. S. Keshavamurthy and W. H. Miller, A Semiclassical Model to Incorporate Multidimensional Tunneling in Classical Trajectory Simulations Using Locally Conserved Actions, *Chem. Phys. Lett.* **205**, 96 (1993).

253. P. Saalfrank and W. H. Miller, Time-Independent Quantum Dynamics for Diatom−Surface Scattering, *J. Chem. Phys.* **98**, 9040 (1993).

254. S. M. Auerbach and W. H. Miller, Quantum Mechanical Reaction Probabilities with a Power Series Green's Function, *J. Chem. Phys.* **98**, 6917 (1993).

255. W. H. Thompson and W. H. Miller, State-Specific Reaction Probabilities from a DVR-ABC Green's Function, *Chem. Phys. Lett.* **206**, 123 (1993).

256. R. Hernandez, W. H. Miller, C. B. Moore, and W. F. Polik, A Random Matrix/Transition State Theory for the Probability Distribution of State-Specific Unimolecular Decay Rates: Generalization to Include Total Angular Momentum Conservation and Other Dynamical Symmetries, *J. Chem. Phys.* **99**, 950 (1993).

257. G. Stock and W. H. Miller, Classical Formulation of the Spectroscopy of Non-Adiabatic Excited-State Dynamics, *J. Chem. Phys.* **99**, 1545 (1993).

258. A. K. Belyaev, D. T. Colbert, G. C. Groenenboom, and W. H. Miller, State-to-State Reaction Probabilities for Processes in $H^-+H_2$, $D_2$ Collisions, *Chem. Phys. Lett.* **209**, 309 (1993).

259. U. Manthe and W. H. Miller, The Cumulative Reaction Probability as Eigenvalue Problem, *J. Chem. Phys.* **99**, 3411 (1993).

260. R. Hernandez and W. H. Miller, Semiclassical Transition State Theory ? A New Perspective, *Chem. Phys. Lett.* **214**, 129 (1993).

261. U. Manthe, T. Seideman, and W. H. Miller, Full Dimensional Quantum Mechanical Calculation of the Rate Constant for the $H_2+OH \rightarrow H_2O+H$ Reaction, *J. Chem. Phys.* **99**, 10078 (1993).

262. C. Leforestier and W. H. Miller, Quantum Mechanical Calculations of the Rate Constant for the Reaction $H+O_2 \rightarrow OH+O$, *J. Chem. Phys.* **100**, 733 (1994).

263. P. Saalfrank and W. H. Miller, Quantum Mechanical Rates for Gas−Surface Processes, *Surf. Sci.* **303**, 206 (1994).

264. S. M. Auerbach and W. H. Miller, Efficient Polynomial Expansion of the Scattering Green's Function: Application to the $D+H_2$ ($\nu=1$) Rate Constant, *J. Chem. Phys.* **100**, 1103 (1994).

265. S. Keshavamurthy and W. H. Miller, Semiclassical Correction for Quantum Mechanical Scattering, *Chem. Phys. Lett.* **218**, 189 (1994).

266. W. H. Miller, Recent Developments in the Quantum Mechanical Theory of Chemical Reaction Rates, in *New Trends in Reaction Rate Theory*, eds. P. Talkner and P. Hänggi, Kluwer Academic Pub., 1995, pp. 225−246.

267. U. Manthe, T. Seideman, and W. H. Miller, Quantum Mechanical Calculations of the Rate Constant for the $H_2+OH \rightarrow H+H_2O$ Reaction: Full Dimensional Results and Comparison to Reduced Dimensionality Problems, *J. Chem. Phys.* **101**, 4759 (1994).

268. W. H. Thompson and W. H. Miller, Initial State-Selected Reaction Probabilities for $OH+H_2 \rightarrow H+H_2O$ and Photodetachment Intensities for $HOH_2^-$, *J. Chem. Phys.* **101**, 8620 (1994).

269. U. Peskin, H. Reisler, and W. H. Miller, On the Relation between Unimolecular Reaction Rates and Overlapping Resonances, *J. Chem. Phys.* **101**, 9672 (1994).

270. G. J. Laming, N. C. Handy, and W. H. Miller, A Comparison of the Gaussian and Bessel Function Exchange for Molecules, *J. Phys. Chem.* **99**, 1880 (1995).

271. U. Peskin and W. H. Miller, Reactive Scattering Theory for Molecular Transitions in Time-Dependent Fields, *J. Chem. Phys.* **102**, 4084 (1995).

272. U. Peskin, W. H. Miller, H. Reisler, Final State-Selected Spectra in Unimolecular Reactions: A Transition-State-Based Random Matrix Model for Overlapping Resonances, *J. Chem. Phys.* **102**, 8874 (1995).

273. W. H. Thompson and W. H. Miller, On the ′Direct′ Calculation of Thermal Rate Constants, *J. Chem. Phys.* **102**, 7409 (1995).

274. W. H. Miller, Quantum Theory of Chemical Reaction Rates, in *Proceedings of the Robert A. Welch Foundation, 38th Conference on Chemical Research, Chemical Dynamics of Transient Species*, (Robert A. Welch Foundation, Houston, TX, 1994) pp. 17−27.

275. J. D. Gezelter and W. H. Miller, Resonant Features in the Energy Dependence of the Rate of Ketene Isomerization, *J. Chem. Phys.* **103**, 7868 (1995).

276. W. H. Miller, Beyond Transition State Theory: Rigorous Quantum Approaches for Determining Chemical Reaction Rates, in *Dynamics of Molecules and Chemical Reactions*, eds. J. Zhang and R. Wyatt, Marcel Dekker, N. Y., 1995, pp. 387−410.

277. W. H. Miller, Quantum Mechanical Theory of Collisional Recombination Rates, *J. Phys. Chem.* **99**, 12387 (1995).

278. U. Peskin, A. Edlund, and W. H. Miller, Quantum Time Evolution in Time-Dependent Fields and Time-Independent Reactive-Scattering Calculations via an Efficient Fourier Grid Preconditioner, *J. Chem. Phys.* **103**, 10030 (1995).

279. W. H. Miller, Quantum Mechanical Theory of Collisional Recombination Rates. Part II. Beyond the Strong Collision Approximation, *Faraday Disk.* **102**, 53 (1995).

280. W. H. Miller, Theoretical Overview of Chemical Dynamics, in *Frontiers of Chemical Dynamics*, ed. E. Yurtsever, NATO ASI Series, Vol. 470, 1995, pp. 1−20.

281. B. W. Spath and W. H. Miller, Semiclassical Calculation of Cumulative Reaction Probabilities, *J. Chem. Phys.* **104**, 95 (1996).

282. L. Lehr and W. H. Miller, A Classical Approach to Dissociative Electron Attachment DA: Application to Temperature Effects in the DA Cross Section of $CF_3$-Cl, *Chem. Phys. Lett.* **250**, 515 (1996).

283. J. D. Gezelter and W. H. Miller, Dynamics of the Photodissociation of Triplet Ketene, *J. Chem. Phys.* **104**, 3546 (1996).

284. V. A. Mandelshtam, H. S. Taylor, and W. H. Miller, Collisional Recombination Reaction $H + O_2 + M \rightarrow HO_2 + M$. Quantum Mechanical Study Using Filter Diagonalization, *J. Chem. Phys.* **105**, 496 (1996).

285. W. H. Thompson, H. O. Karlsson, and W. H. Miller, Theoretical Calculation of Photodetachment Intensities for $H_3O^-$, *J. Chem. Phys.* **105**, 5387 (1996).

286. W. H. Miller, Comment on "Comparison of Positive Flux Operators for Transition State Theory Using a Solvable Model", *J. Chem. Phys.* **105**, 6090 (1996).

287. B. W. Spath and W. H. Miller, Semiclassical Calculation of Franck−Condon Intensities for Reactive Systems, *Chem. Phys. Lett.* **262**, 486 (1996).

288. W. H. Miller, Quantum and Semiclassical Theories of Chemical Reaction Rates, *Adv. Chem. Phys.* **101**, 853 (1997).

289. L. Lehr, J. Manz and W. H. Miller, A Classical Approach to Resonant Low Energy Electron Scattering off Molecules: Application to the $a_1$−Shape Resonance of $CF_3$-Cl, *Chem. Phys.* **214**, 301 (1997).

290. X. Sun and W. H. Miller, Mixed Semiclassical−Classical Approaches to the Dynamics of Complex Molecular Systems, *J. Chem. Phys.* **106**, 916 (1997).

291. W. H. Thompson and W. H. Miller, On the "Direct" Calculation of Thermal Rate Constants. II. The Flux−Flux Autocorrelation Function with Absorbing Potentials, with Application to the $O + HCl \rightarrow OH + Cl$ Reaction, *J. Chem. Phys.* **106**, 142 (1997); Erratum **107**, 2164 (1997).

292. B. Poirier and W. H. Miller, Optimized Preconditioners for Green Function Evaluation in Quantum Reactive Scattering Calculations, *Chem. Phys. Lett.* **265**, 77 (1997).

293. W. H. Miller, Quantum and Semiclassical Green's Functions in Chemical Reaction Dynamics, *J. Chem. Soc. Faraday Trans.* **93**, 685 (1997).

294. U. Peskin, H. Reisler, and W. H. Miller, Response to "Comment on 'On the Relation between Unimolecular Reaction Rates and Overlapping Resonances'", *J. Chem. Phys.* **106**, 4812 (1997).

295. X. Sun and W. H. Miller, Semiclassical Initial Value Representation for Electronically Non-Adiabatic Molecular Dynamics, *J. Chem. Phys.* **106**, 6346 (1997).

296. T. C. Germann and W. H. Miller, Quantum Mechanical Pressure Dependent Reaction and Recombination Rates for $OH+O \rightarrow H+O_2$, $HO_2$, *J. Phys. Chem.* **101**, 6358 (1997).

297. I. Vorobeichik, N. Moiseyev, and W. H. Miller, On the Reflection Probability in Elastic Scattering Processes as obtained via the Absorbing Boundary Conditions−Discrete Variable Representation (ABC-DVR) Green's Function Formalism, *Chem. Phys. Lett.* **275**, 491 (1997).

298. H. Wang, W. H. Thompson, and W. H. Miller, Thermal Rate Constant Using Flux-Flux Autocorrelation Functions: Application to $Cl + H_2 \rightarrow HCl + H$ Reaction, *J. Chem. Phys.* **107**, 7194 (1997).

299. V. S. Batista and W. H. Miller, Semiclassical Molecular Dynamics Simulations of Ultrafast Photodissociation Dynamics Associated with the Chappuis Band of Ozone, *J. Chem. Phys.* **108**, 498 (1998).

300. W. H. Miller, "Direct" and "Correct" Calculation of Microcanonical and Canonical Rate Constants for Chemical Reactions, *J. Phys. Chem.* **102**, 793 (1998).

301. A. Viel, C. Leforestier, and W. H. Miller, Quantum Mechanical Calculation of the Rate Constant for the Reaction $H + O_2 \rightarrow OH + O$, *J. Chem. Phys.* **108**, 3489 (1998).

302. W. H. Miller, Quantum Theory of Chemical Reaction Rates, in *Encyclopedia of Computational Chemistry*, ed. P. v. R. Schleyer, J. Wiley & Sons, Ltd., U.K., Vol. 4, 1998, pp. 2375−2380.

303. W. H. Miller, The Semiclassical Initial Value Representation for Including Quantum Effects in Molecular Dynamics Simulations, in *Classical and Quantum Dynamics in Condensed Phase Simulations*, ed. B. J. Berne, G. Ciccotti, and D. F. Coker, World Scientific, Singapore, 1998, pp. 617−627.

304. X. Sun and W. H. Miller, Semiclassical Initial Value Representation for Rotational Degrees of Freedom: The Tunneling Dynamics of HCl Dimer, *J. Chem. Phys.* **108**, 8870 (1998).

305. W. H. Miller, Quantum Theory of Reactive Scattering and Chemical Reaction Rates, in *Photonic, Electronic, and Atomic Collisions*, ed. F. Aumayr and H. Winter, World Scientific, Singapore, 1998, pp. 441−451.

306. D. E. Skinner, T. C. Germann, and W. H. Miller, Quantum Mechanical Rate Constants for O + OH ↔ H + O$_2$ for Total Angular Momentum J > 0, *J. Phys. Chem.* **102**, 3828 (1998).

307. H. Wang, W. H. Thompson, and W. H. Miller, "Direct" Calculation of Thermal Rate Constants for the F + H$_2$ → HF + H Reaction, *J. Phys. Chem.* **102**, 9372 (1998).

308. H. Wang, X. Sun, and W. H. Miller, Semiclassical Approximations for the Calculation of Thermal Rate Constants for Chemical Reactions in Complex Molecular Systems, *J. Chem. Phys.* **108**, 9726 (1998).

309. T. C. Germann and W. H. Miller, Quantum Mechanical Calculation of Resonance Tunneling in Acetylene Isomerization via the Vinylidene Intermediate, *J. Chem. Phys.* **109**, 94 (1998).

310. X. Sun, H. Wang, and W. H. Miller, On the Semiclassical Description of Quantum Coherence in Thermal Rate Constants, *J. Chem. Phys.* **109**, 4190 (1998).

311. X. Sun, H. Wang, and W. H. Miller, Semiclassical Theory of Electronically Nonadiabatic Dynamics: Results of a Linearized Approximation to the Initial Value Representation, *J. Chem. Phys.* **109**, 7064 (1998).

312. W. H. Miller, Quantum and Semiclassical Theory of Chemical Reaction Rates, *Faraday Disk. Chem. Soc.* **110**, 1 (1998).

313. H. Wang, X. Song, D. Chandler and W. H. Miller, Semiclassical Study of Electronically Nonadiabatic Dynamics in the Condensed-Phase: Spin-Boson Problem with Debye Spectral Density, *J. Chem. Phys.* **110**, 4828 (1999).

314. D. Skinner and W. H. Miller, Application of the Semiclassical Initial Value Representation and Its Linearized Approximation to Inelastic Scattering," *Chem. Phys. Lett.* **300**, 20 (1999).

315. V. S. Batista, M. T. Zanni, B. J. Greenblatt, D. M. Neumark, and W. H. Miller, Femtosecond Photoelectron Spectroscopy of the I$_2^-$ Anion: A Semiclassical Molecular Dynamics Simulation Method, *J. Chem. Phys.* **110**, 3736 (1999).

316. M. T. Zanni, V. S. Batista, B. J. Greenblatt, W. H. Miller, and D. M. Neumark, Femtosecond Photoelectron Spectroscopy of the I$_2^-$ Anion: Characterization of the Ã$'^2'$$_{g,1/2}$ Excited State, *J. Chem. Phys.* **110**, 3748 (1999).

317. X. Sun and W. H. Miller, Forward−Backward Initial Value Representation for Semiclassical Time Correlation Functions, *J. Chem. Phys.* **110**, 6635 (1999).

318. V. Guallar, V. S. Batista and W. H. Miller, Semiclassical Molecular Dynamics Simulations of Excited State Double-Proton Transfer in 7-Azaindole Dimers, *J. Chem. Phys.* **110**, 9922 (1999).

319. H. Wang and W. H. Miller, Analytic Continuation of Real-Time Correlation Functions to Obtain Thermal Rate Constants for Chemical Reaction, *Chem. Phys. Lett.* **307**, 463 (1999).

320. W. H. Miller, Generalization of the Linearized Approximation to the Semiclassical Initial Value Representation for Reactive Flux Correlation Functions, *J. Phys. Chem.* **103**, 9384 (1999).

321. Y. Guo, D. L. Thompson and W. H. Miller, Thermal and Microcanonical Rates of Unimolecular Reactions from an Energy Diffusion Theory Approach, *J. Phys. Chem.* **103**, 10308 (1999).

322. D. E. Skinner and W. H. Miller, Application of the Forward−Backward Initial Value Representation to Molecular Energy Transfer, *J. Chem. Phys.* **111**, 10787 (1999).

323. W. H. Miller, Using Classical Mechanics in a Quantum Framework: Perspective on "Semiclassical Description of Scattering," *Theo. Chem. Acc.* **103**, 236 (2000).

324. H. Wang, M. Thoss, and W. H. Miller, Forward−Backward Initial Value Representation for the Calculation of Thermal Rate Constants for Reactions in Complex Molecular Systems, *J. Chem. Phys.* **112**, 47 (2000).

325. E. A. Coronado, V. S. Batista, and W. H. Miller, Nonadiabatic Photodissociation Dynamics of *ICN* in the Ã Continuum: A Semiclassical Initial Value Representation Study, *J. Chem. Phys.* **112**, 5566 (2000).

326. M. Thoss, W. H. Miller, and G. Stock, Semiclassical Description of Nonadiabatic Quantum Dynamics: Application to the S$_1$−S$_2$ Conical Intersection in Pyrazine, *J. Chem. Phys.* **112**, 10282 (2000).

327. R. Gelabert, X. Gimenez, M. Thoss, H. Wang and W. H. Miller, A Log-Derivative Formulation of the Prefactor for the Semiclassical Herman−Kluk Propagator, *J. Phys. Chem.* **104**, 10321 (2000).

328. V. Guallar, V. S. Batista, and W. H. Miller, Semiclassical Molecular Dynamics Simulations of Intramolecular Proton Transfer in Photoexcited 2-(2′-Hydroxyphenyl-oxazole, *J. Chem. Phys.* **113**, 9510 (2000).

329. V. Guallar, D. Harris, V. S. Batista, G. Loew, and W. H. Miller, A Proton-Transfer Mechanism for Activation of Cytochrome P450eryf, *J. Am. Chem. Soc.* (submitted).

330. R. Gelabert, X. Gimenez, M. Thoss, H. Wang, and W. H. Miller, Semiclassical Description of Diffraction and Its Quenching by the Forward−Backward Version of the Initial Value Representation, *J. Chem. Phys.* **114**, 2572 (2001).

331. H. Wang, M. Thoss, K. Sorge, R. Gelabert, X. Gimenez, and W. H. Miller, Semiclassical Description of Quantum Coherence Effects and Their Quenching: A Forward−Backward Initial Value Representation Study, *J. Chem. Phys.* **114**, 2562 (2001).

332. W. H. Miller, The Semiclassical Initial Value Representation: A Potentially Practical Way for Adding Quantum Effects to Classical Molecular Dynamics Simulations, *J. Phys. Chem.*, in press.

333. M. Thoss, H. Wang, and W. H. Miller, Generalized Forward-Backward Initial Value Representation for the Calculation of Correlation Functions in Complex Systems, *J. Chem. Phys.* (accepted).

334. J. Xing, E. A. Coronado, and W. H. Miller, Some New Classical and Semiclassical Models for Describing Tunneling Processes with Real-Valued Classical Trajectories, *J. Phys. Chem.* (submitted).