

Literaturverzeichnis

- [1] J. Manz and L. Wöste, editors. *Femtosecond Chemistry*. VCH Verlagsgesellschaft, Weinheim, 1995.
- [2] N. Bloembergen and A.H. Zewail. Energy redistribution in isolated molecules and the question of mode-selective chemistry revisited. *J. Phys. Chem.*, 88:5459–5465, 1984.
- [3] C.V. Shank and B.I. Greene. Femtosecond spectroscopy and chemistry. *J. Phys. Chem.*, 87:732–734, 1983.
- [4] A.H. Zewail. Laser femtochemistry. *Science*, 242:1645–1653, 1988.
- [5] L.R. Khundkar and A.H. Zewail. Picosecond photofragment spectroscopy. IV. Dynamics of consecutive bond breakage in the reaction $\text{C}_2\text{F}_4\text{I}_2 \rightarrow \text{C}_2\text{F}_4 + 2 \text{I}$. *J. Chem. Phys.*, 92:231–242, 1990.
- [6] A.H. Zewail. The birth of molecules. *Scientific American*, 263:76–82, 1990.
- [7] A.H. Zewail. Femtosecond transition-state dynamics. In *Structure and Dynamics of Reactive Transition States*, pages 207–237. Faraday Disc. Chem. Soc., 1991. Vol. 91.
- [8] A. H. Zewail. Femtochemistry: Dynamics With Atomic Resolution. In V. Sundström, editor, *Femtochemistry and Femtobiology: Ultrafast Reaction Dynamics at Atomic-Scale Resolution*, pages 1 – 53. Imperial College Press, London, 1997.
- [9] G.K. Paramonov and V.A. Savva. Resonance effects in molecule vibrational excitation by picosecond laser pulses. *Phys. Letters A*, 97:340–342, 1983.

- [10] G.K. Paramonov and V.A. Savva. The effect of state-selective vibrational excitation of an isolated molecule by a picosecond pulse of IR laser radiation. *Izv. Akad. Nauk SSSR, Ser. Fiz.*, 48:449–452, 1984. (in Russian).
- [11] T. Joseph and J. Manz. Mode selective dissociation of vibrationally excited ABA molecular resonances stimulated by a picosecond infrared laser pulse. *Molec. Phys.*, 58:1149–1169, 1986.
- [12] J.E. Combariza, B. Just, J. Manz, and G.K. Paramonov. Isomerizations controlled by ultrashort infrared laser pulses: model simulations for the inversion of ligands (H) in the double-well potential of an organometallic compound, [(C₂H₅)(CO)₂FePH₂]. *J. Phys. Chem.*, 95:10351–10359, 1991.
- [13] B. Just, J. Manz, and G.K. Paramonov. Series of ultrashort infrared laser pulses with analytical shapes for selective vibrational excitation. Model simulations for OH ($v = 0$) \rightarrow OH($v = 10$). *Chem. Phys. Letters*, 193:429–434, 1992.
- [14] M.V. Korolkov, G.K. Paramonov, and B. Schmidt. State-selective control for vibrational excitation and dissociation of diatomic molecules with shaped ultrashort infrared laser pulses. *J. Chem. Phys.*, 105:1862–1879, 1996.
- [15] M.V. Korolkov, J. Manz, and G.K. Paramonov. Theory of ultrafast laser control of isomerization reactions in an environment: picosecond Cope rearrangement of substituted semibullvalenes. *J. Chem. Phys.*, 105:10874–10889, 1996.
- [16] M.V. Korolkov, J. Manz, and G.K. Paramonov. State-selective control for dissipative vibrational dynamics of HOD by shaped ultrashort infrared laser pulses. *J. Phys. Chem.*, 1996. in press.
- [17] M.V. Korolkov, J. Manz, and G.K. Paramonov. Theory of laser control of vibrational transitions and chemical reactions by ultrashort infrared laser pulses. *Adv. Chem. Phys.*, 101, 1997. in press.
- [18] D.J. Tannor, S.A. Rice, and P.M. Weber. Picosecond CARS as a probe of ground electronic state intramolecular vibrational energy redistribution. *J. Chem. Phys.*, 83:6158–6164, 1985.

- [19] D.J. Tannor, R. Kosloff, and S.A. Rice. Coherent pulse sequence induced control of selectivity of reactions: Exact quantum mechanical calculations. *J. Chem. Phys.*, 85:5805–5820, 1986.
- [20] J. Manz. Molecular Wavepacket Dynamics: Theory for Experiments 1926 - 1996. In V. Sundström, editor, *Femtochemistry and Femtobiology: Ultrafast Reaction Dynamics at Atomic-Scale Resolution*, pages 80 – 318. Imperial College Press, London, 1997.
- [21] M.M. Wefers and K.A. Nelson. Ultrafast optical waveforms. *Science*, 262:1381–1382, 1993.
- [22] M.M. Wefers and K.A. Nelson. Programmable phase and amplitude femtosecond pulse shaping. *Opt. Lett.*, 18:2032–2034, 1993.
- [23] H. Kawashima, M.M. Wefers, and K.A. Nelson. Femtosecond pulse shaping, multiple-pulse spectroscopy, and optical control. *Annu. Rev. Phys. Chem.*, 46:627–656, 1995.
- [24] D. Pinkos, J. Squier, D. Schumacher, P. Bucksbaum, B. Kohler, V. V. Yakovlev, and K. R. Wilson. Production of programmable amplified, shaped pulses in femtosecond lasers. In G. A. Mourou, A. H. Zewail, P. F. Barbara, and W. H. Knox, editors, *Ultrafast Phenomena IX*, page 180. Springer, Berlin, 1994.
- [25] M.M. Wefers and K.A. Nelson. Generation of high-fidelity programmable ultrafast optical waveforms. *Opt. Lett.*, 20:1047–1049, 1995.
- [26] M.M. Wefers, K.A. Nelson, and A.M. Weiner. Multidimensional shaping of ultrafast optical waveforms. *Opt. Lett.*, 21:746–748, 1996.
- [27] C.J. Bardeen, V.V. Yakovlev, K.R. Wilson, S.D. Carpenter, P.M. Weber, and W.S. Warren. Feedback quantum control of molecular electronic population transfer. *Chem. Phys. Lett.*, 280:151–158, 1997.
- [28] T. Baumert, J. Helbing, and G. Gerber. Coherent control with femtosecond laser pulses. *Adv. Chem. Phys.*, 101:47, 1997.

- [29] J.G.B. Beumee and H. Rabitz. Robust optimal control theory for selective vibrational excitation in molecules. *J. Chem. Phys.*, 97:1353–1364, 1992.
- [30] R.S. Judson and H. Rabitz. Teaching lasers to molecules. *Phys. Rev. Lett.*, 68:1500, 1992.
- [31] M. Demiralp and H. Rabitz. Optimally controlled quantum molecular dynamics: the effect of nonlinearities on the magnitude and multiplicity of control-field solutions. *Phys. Rev. A*, 47:831, 1993.
- [32] M. Demiralp and H. Rabitz. Optimally controlled quantum molecular dynamics: a perturbation formulation and the existence of multiple solutions. *Phys. Rev. A*, 47:809, 1993.
- [33] J. Botina, H. Rabitz, and N. Rahman. A simplified approach to optimally controlled quantum dynamics. *J. Chem. Phys.*, 104:4031–4040, 1996.
- [34] H. Rabitz. Ramifications of feedback for control of quantum dynamics. volume 101 of *Adv. Chem. Phys. Vol. 101*, page 315. J. Wiley & Sons, New York, 1997.
- [35] W. Zhu, J. Botina, and H. Rabitz. Rapidly convergent iteration methods for quantum optimal control of population. *J. Chem. Phys.*, 108:1953–1963, 1998.
- [36] W. Zhu and H. Rabitz. A rapid monotonically convergent iteration algorithm for quantum optimal control over the expectation value of a positive definite operator. *J. Chem. Phys.*, 109:385–391, 1998.
- [37] M. Oppel. *Quantenchemische und quantendynamische Rechnungen zur Schwingungsanregung und Photodissoziation von HNO₃ durch ultrakurze Laserpulse*. PhD thesis, Freie Universität Berlin, 1998.
- [38] D. R. Hartree. *Proc. Cambridge Phil. Soc.*, 24:111, 1928.
- [39] P. E. M. Siegbahn. The configuration interaction method. In B. O. Roos, editor, *Lecture Notes in Quantum Chemistry*. Springer-Verlag, Berlin, 1992.
- [40] A. Szabo und N. S. Ostlund. *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*. Macmillan Publishing Co., Inc., New-York, 1982.

- [41] M.D. Feit, J.A. Fleck Jr., and A. Steiger. Solution of the Schrödinger equation by a spectral method. *J. Comp. Phys.*, 47:412–433, 1982.
- [42] M.D. Feit and J.A. Fleck Jr. Solution of the Schrödinger equation by a spectral method. II. Vibrational energy levels of triatomic molecules. *J. Chem. Phys.*, 78:301–308, 1983.
- [43] S. Mahapatra and S. Sathyamurthy. Negative imaginary potentials in time dependent quantum molecular scattering. *J. Chem. Soc. Faraday Trans.*, 93:773, 1997.
- [44] J.W. Cooley and J.W. Tukey. An algorithm for the machine calculation of complex Fourier series. *Math. Comp.*, 19:297–301, 1965.
- [45] D. Kosloff and R. Kosloff. A Fourier method solution for the time dependent Schrödinger equation as a tool in molecular dynamics. *J. Comp. Phys.*, 52:35–53, 1983.
- [46] R. Kosloff and D. Kosloff. A Fourier method solution for the time dependent Schrödinger equation: A study of the reaction $H^+ + H_2$, $D^+ + D_2$, and $D^+ + H_2$. *J. Chem. Phys.*, 79:1823–1833, 1983.
- [47] C. Leforestier, R.H. Bisseling, C. Cerjan, M.D. Feit, R. Friesner, A. Guldberg, A. Hammerich, G. Jolicard, W. Karrlein, H.-D. Meyer, N. Lipkin, O. Roncero, and R. Kosloff. A comparison of different propagation schemes for the time dependent Schrödinger equation. *J. Comp. Phys.*, 94:59–80, 1991.
- [48] R. Kosloff. Time-dependent quantum-mechanical methods for molecular dynamics. *J. Phys. Chem.*, 92:2087–2100, 1988.
- [49] J. Alvarellos and H. Metiu. The evolution of a wave function in a curve crossing problem computed by a Fast-Fourier-Transform method. *J. Chem. Phys.*, 88:4957, 1988.
- [50] A.D. Bandrauk and H. Shen. Higher order exponential split operator method for solving time-dependent Schrödinger equations. *Can. J. Chem.*, 70:555–559, 1992.

- [51] A.D. Bandrauk and H. Shen. Exponential split operator methods for solving coupled time-dependent Schrödinger equations. *J. Chem. Phys.*, 99:1185–1193, 1993.
- [52] B. Reischl. Quantum dynamical three-dimensional ab initio approach to a femtosecond pump-probe ionization spectrum of $\text{Na}_3(\text{B})$ at low laser field intensities. *Chem. Phys. Lett.*, 239:173–180, 1995.
- [53] R. Car and M. Parinello. Unified approach for molecular dynamics and density-functional theory. *Phys. Rev. Lett.*, 55:2471 – 2474, 1985.
- [54] BSP-Libraries erhältlich über <http://www.bsp-worldwide.org>.
- [55] R.H. Bisseling and W.F. McColl. Scientific computing on bulk synchronous parallel architectures, Vol. I. In B. Pehrson and I. Simon, editors, *Proc. IFIP 13th World Computer Congress*, pages 509–514, North-Holland, 1994.
- [56] W. F. McColl. Scalable computing. In J van Leeuwen, editor, *Computer Science Today: Recent Trends and Developments, number 1000 in Lecture notes in Computer Science*, pages 41 – 61. Springer-Verlag, Berlin, 1996.
- [57] L.G. Valiant. A bridging model for parallel computation. *Communications of the ACM*, 8:103–111, 1990.
- [58] R. Bisseling. Basic techniques for numerical linear algebra on bulk synchronous parallel computers. In L. Vulkov, J. Wasniewski, and P. Yalamov, editors, *Proc. First Workshop on Numerical Analysis and Applications, Rousse, Bulgaria 1996, Lecture Notes in Computer Science*, volume 1196, pages 45 – 57, Berlin, 1996. Springer-Verlag.
- [59] T. Beth. *Verfahren der schnellen Fourier Transformation*. Teubner, Stuttgart, 1984.
- [60] D.J. Tannor and S.A. Rice. Control of selectivity of chemical reaction via control of wave packet evolution. *J. Chem. Phys.*, 83:5013–5018, 1985.
- [61] A.H. Zewail. Femtochemistry: chemical reaction dynamics and their control. *Adv. Chem. Phys.*, 101:3, 1997.

- [62] T. Baumert and G. Gerber. Fundamental interactions of molecules (Na_2 , Na_3) with intense femtosecond laser pulses. *Israel J. Chem.*, 34:103–114, 1994.
- [63] W. Jakubetz, J. Manz, and H.-J. Schreier. Theory of optimal laser pulses for selective transitions between molecular eigenstates. *Chem. Phys. Lett.*, 165:100–106, 1990.
- [64] J. Cao, M. Messina, and K. R. Wilson. Quantum control of dissipative systems: Exact solutions. *J. Chem. Phys.*, 106:5239, 1998.
- [65] C. J. Bardeen, V. V. Yakovlev, K. R. Wilson, S. D. Carpenter, P. M. Weber, and W. S. Warren. Feedback quantum control of population transfer using shaped femtosecond pulses. In T. Elsaesser, J. G. Fujimoto, D. Wiersma, and W. Zinth, editors, *Ultrafast Phenomena XI*. Springer-Verlag, Berlin, 1998. to be published.
- [66] *Brockhaus Enzyklopädie, 17. Ausgabe*. F. A. Brockhaus, Wiesbaden, 1974.
- [67] H. Heuser. *Lehrbuch der Analysis, Teil 2*. B. G. Teubner, Stuttgart, 1988.
- [68] H. Heuser. *Funktionalanalysis*. B. G. Teubner, Stuttgart, 1986.
- [69] M. Reed and B. Simon. *Methods of Modern Mathematical Physics. I: Functional Analysis*. Academic Press, New York, 1972.
- [70] D. H. Lieb and B. Simon. The hartree-fock theory for coulomb systems. *Commun. math. Phys.*, 53:185 – 194, 1977.
- [71] A.M. Weiner, D.E. Leaird, J.S. Patel, and J.R. Wull. Femtosecond laser pulse shaping by use of microsecond radio-frequency pulses. *Opt. Lett.*, 15:326, 1990.
- [72] C.W. Hillegas, J.X. Tull, D. Goswami, D. Strickland, and W.S. Warren. Programmable femtosecond pulse shaping by use of a multielement liquid-crystal phase modulator. *Opt. Lett.*, 19:737, 1994.
- [73] J. Gaus. *Strukturelle und elektronische Eigenschaften kleiner reiner, gemischter und dotierter Alkalimetall-Cluster*. PhD thesis, Freie Universität Berlin, 1995.

- [74] J. Gaus, K. Kobe, V. Bonačić-Koutecký, H. Kühling, J. Manz, B. Reischl, S. Rutz, E. Schreiber, and L. Wöste. Experimental and theoretical approach to the pseudorotating $\text{Na}_3(\text{B})$. *J. Chem. Phys.*, 97:12509–12515, 1993.
- [75] R. de Vivie-Riedle, B. Reischl, S. Rutz, and E. Schreiber. Femtosecond study of multiphoton ionization processes in K_2 at moderate laser intensities. *J. Phys. Chem.*, 99:16829–16834, 1995.
- [76] S. Rutz, R. de Vivie-Riedle, and E. Schreiber. Femtosecond wave-packet propagation in spin-orbit-coupled electronic states of $^{39,39}\text{K}_2$ and $^{39,41}\text{K}_2$. *Phys. Rev. A*, 54:306–313, 1996.
- [77] R. de Vivie-Riedle, K. Kobe, J. Manz, W. Meyer, B. Reischl, S. Rutz, E. Schreiber, and L. Wöste. Femtosecond study of multiphoton ionization processes in K_2 : From pump-probe to control. *J. Phys. Chem.*, 100:7789–7796, 1996.
- [78] R. de Vivie-Riedle, J. Gaus, V. Bonačić-Koutecký, J. Manz, B. Reischl, S. Rutz, E. Schreiber, and L. Wöste. Pulse width controlled molecular dynamics: Symmetric stretch versus pseudorotations in $\text{Na}_3(\text{B})$. In M. Chergui, editor, *Femtochemistry*, pages 319–326. World Scientific, Singapore, 1996.
- [79] R.S. Berry, V. Bonačić-Koutecký, J. Gaus, T. Leisner, J. Manz, B. Reischl-Lenz, H. Ruppe, S. Rutz, E. Schreiber, S. Vajda, R. de Vivie-Riedle, S. Wolf, and L. Wöste. Size dependent ultrafast relaxation phenomena in metal clusters. *Adv. Chem. Phys.*, 101:101 – 139, 1997.
- [80] R. de Vivie-Riedle, J. Gaus, V. Bonačić-Koutecký, J. Manz, B. Reischl-Lenz, and P. Saalfrank. Theoretical study of the absorption spectrum of the pseudorotating $\text{Na}_3(\text{B})$. *Chem. Phys.*, 223:1 – 14, 1997.
- [81] MOLPRO is a package of ab initio programs written by H.-J. Werner and P. J. Knowles, with contributions from J. Almlöf, R. D. Amos, A. Berning, M. J. O. Deegan, F. Eckert, S. T. Elbert, C. Hampel, R. Lindh, W. Meyer, A. Nicklass, K. Peterson, R. Pitzer, A. J. Stone, P. R. Taylor, M. E. Mura, P. Pulay, M. Schütz, H. Stoll, T. Thorsteinsson, and D. L. Cooper.

- [82] D. Neuhauser. Circumventing the Heisenberg principle: A rigorous demonstration of filter-diagonalization on a LiCN model. *J. Chem. Phys.*, 100:5076 – 5079, 1994.
- [83] J. Manz, K. Sundermann, and R. de Vivie-Riedle. Quantum optimal control strategies for photoisomerization via electronically excited states. *Chem. Phys. Lett.*, 290:415 – 422, 1998.
- [84] H. Tal-Ezer und R. Kosloff. A direct relaxation method for calculating eigenfunctions and eigenvalues of the Schrödinger equation. *Chem. Phys. Lett.*, 127:223 – 230, 1986.
- [85] P. Saalfrank, private Mitteilung, FUB, 1998.
- [86] P. Schuster, G. Zundel, and C. Sandorfy, editors. *The Hydrogen Bond*. North Holland Publ. Co., Amsterdam, 1976.
- [87] G. A. Jeffrey and W. Saenger. *Hydrogen Bonding in Biological Structures*. Springer, Berlin, 1991.
- [88] Hans-Heinrich Limbach and J. Manz. Hydrogen Transfer: Theory and Experiment. *Ber. Bunsenges. Phys. Chem.*, 102:289 – 291, 1998.
- [89] A. Douhal, S.K. Kim, and A.H. Zewail. Femtosecond molecular dynamics of tautomerization in model base pairs. *Nature*, 378:260, 1995.
- [90] A. Douhal, F. Lahmani, and A.H. Zewail. Proton-transfer reaction dynamics. *Chem. Phys.*, 207:477–498, 1996.
- [91] N. Makri and W.H. Miller. Time-dependent self-consistent field (TDSCF) approximation for a reaction coordinate coupled to a harmonic bath: Single and multiple configuration treatments. *J. Chem. Phys.*, 87:5781–5787, 1987.
- [92] L. González, O. Mó, and M. Yáñez. High level ab initio calculations on the intramolecular hydrogen bond in thiomalonaldehyde. *J. Phys. Chem. A*, 101:9710, 1997.
- [93] B. A. Ruf and W. H. Miller. A new (cartesian) reaction-path model for dynamics in polyatomic systems, with application to H-atom transfer in malonaldehyde. *J. Chem. Soc*, 84:1523 – 1534, 1988.

- [94] O. Kühn, private Mitteilung, FUB, 1998.
- [95] N. Došlić, O. Kühn, and J. Manz. A. Coherent vs. incoherent hydrogen dynamics across or through a barrier. *Ber. Bunsenges. Phys. Chem.*, 102:292 – 297, 1998.
- [96] M. Dohle, J. Manz, G.K. Paramonov, and H. Quast. Design of substituted semibullvalenes suitable for control of the Cope rearrangement by two ps IR laser pulses. *Chem. Phys.*, 197:91–97, 1995.
- [97] L.V. Keldysh. Ionization in the field of a strong electromagnetic wave. *Sov. Phys. JETP*, 20:1307–1314, 1965.
- [98] N. Došlić, private Mitteilung, FUB, 1998.
- [99] N. Došlić, O. Kühn, J. Manz, and K. Sundermann. The "Hydrogen-Subway" a tunneling approach to intramolecular hydrogen transfer reactions controlled by ultrashort laser pulses. *J. Phys. Chem.*, 1998. accepted.
- [100] H. Naundorf, O. Kühn, and K. Sundermann. Laser driven hydrogen tunneling in a dissipative environment. *J. Chem. Phys.*, 1998. submitted.
- [101] M. Demiralp and H. Rabitz. Assessing optimality and robustness of control over quantum dynamics. *Phys. Rev. A*, 57:2420 – 2471, 1998.
- [102] R. Marquardt and M. Quack. Radiative excitation of the harmonic oscillator with applications to stereomutation in chiral molecules. *Z. Physik D*, 36:229–237, 1996.
- [103] K. Bergmann and B.W. Shore. Coherent population transfer. In H.-L. Dai and R.W. Field, editors, *Molecular dynamics and spectroscopy by stimulated emission pumping*, Advanced Series in Physical Chemistry – Vol. 4, pages 315–373, Singapore, 1995. World Scientific.
- [104] A. M. Weiner. Femtosecond optical pulse shaping and processing. *Prog. Quant. Electr.*, 19:161 – 237, 1995.
- [105] J. X. Tull, M. A. Dugan, and W. S. Warren. High-resolution, ultrafast laser pulse shaping and its applications. *Advances in Magnetic and Optical Resonance*, 20:1 –65, 1997.

-
- [106] C. C. Marston and G. Balint-Kurti. The Fourier grid Hamiltonian method for bound state eigenvalues and eigenfunctions. *J. Chem. Phys.*, 91:3571 – 3576, 1989.
- [107] A. S. Dickinson and P. R. Certain. Calculation of matrix elements for one-dimensional quantum-mechanical problems. *J. Chem. Phys.*, 49:4209, 1968.
- [108] J. C. Light, I. P. Hamilton, and J. V. Lill. Generalized discrete variable approximation in quantum mechanics. *J. Chem. Phys.*, 82:1400, 1985.
- [109] D. Neuhauser. Bound state eigenfunctions from wave packets: Time \rightarrow energy resolution. *J. Chem. Phys.*, 93:2611 – 2616, 1990.
- [110] R. Chen and H. Guo. A general and efficient filter-diagonalization method without time propagation. *J. Chem. Phys.*, 105:1311 – 1317, 1996.