Bibliography

[1] G. Ertl. *Elementarschritte bei der heterogenen Katalyse*. Angew. Chem., **102**:1258–1266 (1990).

[2] R. Schuster, V. Kirchner, X. H. Xia, A. M. Bittner, and G. Ertl. *Nanoscale Electrochemistry*. Phys. Rev. Lett., **80**:5599–5602 (1998).

[3] J. Manz. *Molecular wavepacket dynamics: Theory for experiments 1926-1996*. In V. Sundström, ed., *Femtochemistry and Femtobiology*. World Scientific, Singapore (1997).

[4] M. Dantus, M. J. Rosker, and A. H. Zewail. *Real-time femtosecond probing of "transition states" in chemical reactions*. J. Chem. Phys., **87**:2395–2397 (1987).

[5] T. S. Rose, M. J. Rosker, and A. H. Zewail. *Femtosecond real-time observation of wave packet oscillations (resonance) in dissociation reactions*. J. Chem. Phys., **88**:6672–6673 (1988).

[6] A. Gross, S. Wilke, and M. Scheffler. *Six-dimensional Quantum Dynamics of Adsorption and Desorption of H_2 at Pd(100): Steering and Steric Effects*. Phys. Rev. Lett., **75**:2718–2721 (1995).

[7] G. J. Kroes, E. J. Baerends, and R. C. Mowrey. *Six-dimensional Quantum Dynamics of Dissociative Chemisorption of ($v = 0$, $j = 0$) H_2 at Cu(100)*. Phys. Rev. Lett., **78**:3583–3586 (1997).

[8] J. Dai and J. C. Light. *Six Dimensional Quantum Dynamics Study for Dissociative Adsorption of H_2 on Cu(111) Surface*. J. Chem. Phys., **107**:1676–1679 (1997).

[9] L. A. Peterman. *Thermal Desorption Kinetics of Chemisorbed Gases*. Progr. in Surf. Sci., **1**:2–61 (1972).

[10] J. C. Tully, M. Gomez, and M. Head-Gordon. *Electronic and Phonon Mechanisms of Vibrational Relaxation: CO on Cu(100)*. J. Vac. Sci. Technol. A, **11**:1914–1920 (1993).

[11] M. Dohle and P. Saalfrank. *Surface oscillator models for dissociative sticking of molecular hydrogen at non-rigid surfaces*. Surf. Sci., **373**:95–108 (1997).

[12] H. Guo, P. Saalfrank, and T. Seideman. *Theory of photoinduced surface reactions of admolecules*. Progr. in Surf. Sci., **62**:239–303 (1999).

[13] P. Saalfrank, G. Boendgen, K. Finger, and L. Pesce. *Photodesorption of NO from a metal surface: quantum dynamical implications of a two-mode model*. Chem. Phys., **251**:51–69 (2000).

[14] J. Boh, G. Eilmsteiner, K. D. Rendulic, and A. Winkler. *Adsorption and abstraction of atomic hydrogen (deuterium) on Al(100)*. Surf. Sci., **395**:98–110 (1998).

[15] V. May and O. Kühn. *Charge and Energy Transfer Dynamics in Molecular Systems*. WILEY-VCH, Berlin, 1st edn. (2000).

[16] I. L. Shumay, U. Höfer, C. Reuß, U. Thomann, W. Wallauer, and T. Fauster. *Lifetimes of image-potential states on Cu(100) and Ag(100) measured by femtosecond time resolved two-photon photoemission*. Phys. Rev. B, **58**:13974–13981 (1998).

[17] U. Höfer, I. L. Shumay, C. Reuß, U. Thomann, and W. Wallauer. *Time-Resolved Choerent Photoelectron Spectroscopy of Quantized Electronic States on Metal Surfaces*. Science, **277**:1480–1482 (1997).

[18] T. Fauster, C. Reuß, I. L. Shumay, and M. Weinelt. *Femtosecond two-photon photoemission studies of image-potential states*. Chem. Phys., **251**:111–121 (2000).

[19] T. Klamroth and P. Saalfrank. *Effect of substrate vibrations on the sticking of atoms at surfaces: A critical comparison of different propagation methods for the H/Cu(100) system*. J. Chem. Phys., **112**:10571–10581 (2000).

[20] K. Christmann. *Interaction of Hydrogen with Solid Surfaces*. Surf. Sci. Repts., **9**:1–164 (1988).

[21] D. Shalashilin, B. Jackson, and M. Persson. *Eley-Rideal and hot-atom dynamics of HD formation by H(D) incident from the gas phase on D(H)-covered Cu(111)*. Faraday Discuss., **110**:287–300 (1998).

[22] J. Harris and B. Kasemo. *The water reaction on Platinum: An example of a precursor mechanism ?*. Surf. Sci., **105**:281–290 (1981).

[23] C. L. Lamont, B. N. J. Persson, and G. P. Williams. *Dynamics of atomic adsorbates: Hydrogen on Cu(111)*. Chem. Phys. Lett., **243**:429–434 (1995).

[24] U. Bischler, P. Sandl, E. Bertel, T. Brunner, and W. Brenig. *Sticking, Adsorption, and Absorption of Atomic H on Cu(110)*. Phys. Rev. Lett., **70**:3603–3606 (1993).

[25] K. Schönhammer and O. Gunnarsson. *Sticking and inelastic scattering at metal surfaces: The electron-hole pair mechanism*. Surf. Sci., **117**:53–59 (1984).

[26] B. N. J. Persson and M. Persson. *Vibrational lifetime for CO adsorbed on Cu(100)*. Solid State Commun., **36**:175–179 (1980).

[27] J. W. Gadzuk. *A dissipative trajectory theory for reactive scattering at surfaces*. Surf. Sci., **118**:180–192 (1982).

[28] B. N. J. Persson and J. W. Gadzuk. *Comments on vibrational dynamics of low-frequency adsorbate motion*. Surf. Sci. Lett., **410**:779–782 (1998).

[29] G. P. Brivio and T. B. Grimley. *Non-adiabatic processes in adsorption/desorption phenomena*. Surf. Sci., **89**:226–237 (1979).

[30] G. D. Billing. *Semiclassical Formulation of Molecule Surface Scattering Using an Embedded Diatomics in Molecules Potential*. Chem. Phys., **99**:15378–15386 (1995).

[31] G. Borisov, A. K. Kazansky, and J. P. Gauyacq. *Resonant charge transfer in ion-metal surface collisions: Effects of a projected band gap in the H^--Cu(111) system*. Phys. Rev. B, **59**:10935–10949 (1999).

[32] S. Gao. *Quantum kinetic theory of vibrational heating and bond breaking by hot electrons*. Phys. Rev. B, **55**:1876–1886 (1997).

[33] J. C. Tully. *Dynamics of Chemical Processes at Surfaces*. Acc. Chem. Res., **14**:188–193 (1981). And references therein.

[34] D. V. Shalashilin and B. Jackson. *Formation and dynamics of hot-precursor atoms on metal surfaces: Trajectory simulations and stochastic models*. J. Chem. Phys., **109**:2856–2864 (1998).

[35] M. Hand and J. Harris. *Recoil effects in surface dissociation*. J. Chem. Phys., **92**:7610–7617 (1990).

[36] R. Baer and R. Kosloff. *Quantum dissipative dynamics of adsorbates near metal surfaces: A surrogate hamiltonian theory applied to hydrogen on nickel*. J. Chem. Phys., **106**:8862–8875 (1997).

[37] N. Makri and W. H. Miller. *Time-dependent self-consistent field (TD-SCF) approximation for a reaction coordinate coupled to a harmonic bath: Single and multiple configuration treatments*. J. Chem. Phys., **87**:5781–5787 (1987).

[38] H.-D. Meyer, U. Manthe, and L. S. Cederbaum. *The multi-configurational time-dependent Hartree approach*. Chem. Phys. Lett., **165**:73–78 (1990).

[39] B. Jackson. *Quantum semiclassical calculations of gas-surface energy transfer and sticking*. Comp. Phys. Commun., **80**:119–144 (1994).

[40] K. Blum. *Density matrix theory and applications*. Plenum Press, New York (1981).

[41] B. Jackson. *Dissociative adsorption at finite temperature: Multiconfiguration vector description of the reduced density matrix*. Chem. Phys. Lett., **308**:456–462 (1999).

[42] S. Y. Guan, J. T. Muckerman, and T. Uzer. *Desorption of vibrationally excited adsorbates in competition with relaxation: A quantal picture*. J. Chem. Phys., **93**:4400–4412 (1990). For example.

[43] D. S. Sholl and J. C. Tully. *A generalized surface hopping method*. J. Chem. Phys., **109**:7702–7710 (1998). And references therein.

[44] M. S. Daw and M. I. Baskes. *Semiempirical, Quantum Mechanical Calculation of Hydrogen Embrittlement in Metals*. Phys. Rev. Lett., **50**:1285–1288 (1983).

[45] M. S. Daw and M. I. Baskes. *Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals*. Phys. Rev. B, **29**:6643–6652 (1984).

[46] K. W. Jacobsen, P. Stolze, and J. K. Nørskov. *A semi-empirical effective medium theory for metals and alloys*. Surf. Sci., **366**:394–402 (1996).

[47] M. J. Stott and E. Zaremba. *Quasiatoms: An approach to atoms in nonuniform electronic systems*. Phys. Rev. B, **22**:1564–1583 (1980).

[48] P. Hohenberg and W. Kohn. *Inhomogeneous Electron Gas*. Phys. Rev., **136B**:864–871 (1964).

[49] J. Strömquist, L. Bengtsson, M. Persson, and B. Hammer. *The dynamics of H absorption in and adsorption on Cu(100)*. Surf. Sci., **387**:382–394 (1998).

[50] M. D. Feit, J. F. Jr., and A. Steiger. *Solution of the Schrödinger equation by a spectral method*. J. Comput. Phys., **47**:412–433 (1982).

[51] G. Jolicard and G. D. Billing. *Energy dependence of vibrational inelastic collisions using the wave operator theory and an analysis of quantum flows in momentum space*. Chem. Phys., **149**:261–273 (1991).

[52] J.-Y. Ge and J. Z. H. Zhang. *Use of negative complex potential as absorbing potential*. J. Chem. Phys., **108**:1429–1433 (1998).

[53] U. V. Riss and H.-D. Meyer. *Investigation on the reflection and transmission properties of complex absorbing potentials*. J. Chem. Phys., **105**:1409–1419 (1996).

[54] F. A. Bornemann, P. Nettesheim, and C. Schütte. *Quantum-classical molecular dynamics as an approximation to full quantum dynamics*. J. Chem. Phys., **105**:1074–1083 (1996).

[55] IEEE, New York. *ANSI/IEEE Std 754-1985, IEEE Standard for Binary Floating-Point Arithmetic* (1985).

[56] P. Nettesheim, F. A. Bornemann, B. Schmidt, and C. Schütte. *An explicit and symplectic integrator for quantum-classical molecular dynamics*. Chem. Phys. Lett., **256**:581–588 (1996).

[57] U. Peskin and M. Steinberg. *A temperature-dependent Schrödinger equation based on a time-dependent self consistent field approximation*. J. Chem. Phys., **109**:704–710 (1998).

[58] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery. *Numerical Recipes*. Cambridge University Press, Cambridge, second edn. (1992).

[59] H.-W. Lee. *Theory and application of the quantum phase-space distribution functions*. Physics Repts., **259**:147–211 (1995).

[60] R. A. Olsen, G. J. Kroes, and E. J. Baerends. *The influence of molecular rotation on the direct subsurface absorption of H_2 on Pd(111)*. J. Chem. Phys., **109**:2450–2459 (1998).

[61] D. C. Harris, G. R. Darling, and S. Holloway. *Analysis of a semiquantal method for molecular dynamics*. Surf. Sci., **433-435**:838–842 (1999).

[62] M. Dohle, T. Uzer, and P. Saalfrank. *The dissociation of diatomic molecules on vibrating surfaces: A semiclassical generalized Langevin approach*. J. Chem. Phys., **108**:4226–4236 (1998).

[63] P. Jungwirth and R. B. Gerber. *Quantum Molecular Dynamics of Ultrafast Processes in Large Polyatomic Systems*. Chem. Rev., **99**:1583–1606 (1999).

[64] J. O. Jung and R. B. Gerber. *Vibrational wave functions and spectroscopy of $(H_2O)_n$, n =2,3,4,5: Vibrational self-consistent field with correlation corrections*. J. Chem. Phys., **105**:10332–10348 (1996).

[65] J. T. Kindt, J. C. Tully, M. Head-Gordon, and M. A. Gomez. *Electron-hole pair contributions to scattering, sticking and surface diffusion: CO on Cu(100)*. J. Chem. Phys., **109**:3629–3636 (1998).

[66] 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**:9922–9936 (1999). And references therein.

[67] M. Topaler and N. Makri. *Quantum rates for a double well coupled to a dissipative bath: Accurate path integral results and comparison with approximate theories*. J. Chem. Phys., **101**:7500–7519 (1994).

[68] R. B. Gerber. *Molecular Scattering from Surfaces: Theoretical Methods and Results*. Chem. Rev., **87**:29–79 (1987).

[69] G. Benedek and N. Garcia. *Inelastic Scattering of He from LiF(001) Surface: Theoretical Analysis of Time-of-Flight Spectra*. Surf. Sci. Lett., **103**:143–148 (1981).

[70] A. Bilić and B. Gumhalter. *Quantum versus semiclassical treatment of multiphonon effects in He-atom scattering from surfaces*. Phys. Rev. B, **52**:12307–12328 (1995).

[71] B. Gumhalter and D. C. Langreth. *Unified model of diffractive and multiphonon He atom scattering from adsorbates: Holstein renormalization of the interactions and the complete Debye-Waller factor*. Phys. Rev. B, **60**:2789–2809 (1999).

[72] H. Schlichting, D. Menzel, T. Brunner, and W. Brenig. *Sticking of rare gas atoms on the clean Ru(001) surface*. J. Chem. Phys., **97**:4453–4467 (1992).

[73] I. E. Tamm. *Über eine mögliche Art der Elektronenbindung an Kristalloberflächen*. Z. Phys., **76**:849–852 (1932).

[74] W. Shockley. *On the Surfaces States Associated with a Periodic Potential*. Phys. Rev., **56**:317–323 (1939).

[75] P. M. Echenique and J. B. Pendry. *The existence and detection of Rydberg states at surfaces*. J. Phys. C., **11**:2065–2075 (1978).

[76] D. Straub, W. Altmann, H. Scheidt, and V. Dose. *Summary Abstract: Intrinsic unoccupied surfaces states at GaP(110)*. J. Vac. Sci. Technol. A, **2**:529–530 (1984).

[77] V. Dose, W. Altmann, A. Goldmann, U. Kolac, and J. Rogozik. *Image-Potential States observed by Inverse Photoemission*. Phys Rev. Lett., **52**:1919–1921 (1984).

[78] P. M. Echenique, J. M. Pitarke, E. V. Chulkov, and A. Rubio. *Theory of inelastic lifetimes of low-energy electrons in metals*. Chem. Phys., **251**:1–25 (2000).

[79] P. M. Echenique and J. B. Pendry. *Theory of Image States at Metal Surfaces*. Prog. Surf. Sci., **32**:111–172 (1989).

[80] G. Borstel and G. Thörner. *Inverse photoemission from solids: Theoretical aspects and applications*. Surf. Sci. Rep., **8**:1–41 (1988).

[81] S. L. Hulbert, P. D. Johnson, M. Weinert, and R. F. Garrett. *Unoccupied surface states on Cu(001): A comparison of experiment and theory*. Phys. Rev. B, **33**:760–764 (1986).

[82] S. Papadia, M. Persson, and L.-A. Salmi. *Image-potential-induced resonances at free-electron-like metal surfaces*. Phys. Rev. B, **41**:10237–10239 (1990).

[83] M. Nekovee, S. Crampin, and J. E. Inglesfield. *Magnetic splitting of image states at Fe(110)*. Phys. Rev. Lett., **70**:3099–3102 (1993).

[84] T. Fondén, S. Papadia, and M. Persson. *Scanning tunneling spectroscopy of unoccupied surface resonances at free-electron-like metal surfaces*. J. Phys. Condens. Matter, **7**:2697–2716 (1995).

[85] N. V. Smith. *Phase analysis of image states and surface states associated with nearly-free-electron band gaps*. Phys. Rev. B., **32**:3549–3555 (1985).

[86] T. Fauster. *Calculation of surface states using a one-dimensional scattering model*. Appl. Phys. A, **59**:639–643 (1994).

[87] V. M. Silkin and E. V. Chulkov. *State of the image potential on Al(001), Al(111), an Al(001) + c(2x2)Na surfaces*. Phys. Solid State, **36**:404–409 (1994).

[88] Z. Li and S. Gao. *Band-theory calculation of image states on a metal surface*. Phys. Rev. B, **50**:15349–15352 (1994).

[89] E. V. Chulkov, V. M. Silkin, and P. M. Echenique. *Image potential states on metal surfaces: binding energies and wave functions*. Surf. Sci., **437**:330–352 (1999).

[90] P. M. Echenique, F. Flores, and F. Sols. *Lifetime of image surface states*. Phys. Rev. Lett., **55**:2348–2350 (1985).

[91] P. L. de Andrés, P. M. Echenique, and F. Flores. *Lifetimes in a two-dimensional image-potential-induced electron band*. Phys. Rev. B, **35**:4529–4532 (1987).

[92] P. L. de Andrés, P. M. Echenique, and F. Flores. *Calculation of the lifetimes for intermediate Rydberg states*. Phys. Rev. B, **39**:10356–10358 (1989).

[93] M. E. Uranga, A. Rivacoba, and P. M. Echenique. *Image States: Idea and Theoretical Development*. Progr. Surf. Sci., **42**:67–74 (1993).

[94] F. J. Himpsel. *Inverse Photoemission*. Comments Cond. Matter Phys., **12**:199 (1986).

[95] N. V. Smith. *Inverse photoemission*. Rep. Prog. Phys., **51**:1227–1294 (1988).

[96] A. Goldmann, V. Dose, and G. Borstel. *Empty electronic states at the (100), (110), and (111) surfaces of nickel, copper, and silver*. Phys. Rev. B, **32**:1971–1980 (1985).

[97] F. J. Himpsel and J. E. Ortega. *Electronic structure of Cu(100), Ag(100), Au(100), and Cu_3Au(100) from inverse photoemission*. Phys. Rev. B, **46**:9719–9723 (1992).

[98] M. Donath. *Spin-dependent electronic structure at magnetic surfaces: the low-Miller-index surfaces of nickel*. Surf. Sci. Rep., **20**:251–316 (1994).

[99] K. Giesen, F. Hage, F. J. Himpsel, H. J. Riess, and W. Steinmann. *Two-photon photoemission via image-potential states*. Phys. Rev. Lett., **55**:300–303 (1985).

[100] W. Merry, R. E. Jordan, D. E. Padowitz, and C. B. Harris. *Electrons at metal-insulator interfaces*. Surf. Sci., **295**:293–401 (1993).

[101] T. Fauster and W. Steinmann. *Two-photon photoemission spectroscopy of image states*. In P. Halevi, ed., *Photonic Probes of Surfaces*, chap. 8, 347. Elsevier, Amsterdam (1995).

[102] G. Binnig, K. H. Frank, H. Fuchs, N. Garcia, B. Reihl, H. Rohrer, F. Salvan, and A. R. Williams. *Tunneling Spectroscopy and Inverse Photoemission: Image and Field States*. Phys. Rev. Lett., **55**:991–994 (1985).

[103] R. W. Schoenlein, J. G. Fujimoto, G. L. Eesley, and T. W. Capehart. *Femtosecond relaxation dynamics of image-potential states*. Phys. Rev. B, **43**:4688–4698 (1991).

[104] R. W. Schoenlein, J. G. Fujimoto, G. L. Eesley, and T. W. Capehart. *Femtosecond dynamics of the n=2 image-potential state on Ag(100)*. Phys. Rev. B, **41**:5436–5439 (1990).

[105] R. W. Schoenlein, J. G. Fujimoto, G. L. Eesley, and T. W. Capehart. *Femtosecond studies of image-potential dynamics in metals*. Phys. Rev. Lett., **61**:2596–2599 (1988).

[106] T. Hertel, E. Knoesel, M. Wolf, and G. Ertl. *Ultrafast electron dynamics at Cu(111): Response of an electron gas to optical excitation*. Phys. Rev. Lett., **76**:535–538 (1996).

[107] E. Knoesel, T. Hertel, M. Wolf, and G. Ertl. *Femtosecond dynamics of electronic excitations of adsorbates studied by two-photon photoemission pulse correlation: CO/Cu(111)*. Chem. Phys. Lett., **240**:409–416 (1995).

[108] M. Wolf, E. Knoesel, and T. Hertel. *Ultrafast dynamics of electrons in image-potential states on clean and Xe-covered Cu(111)*. Phys. Ref. B, **54**:5295–5298 (1996).

[109] U. Höfer. *Dynamik von Bildladungszuständen*. In *Femtosekunden und Nano-eV: Dynamik in kondensierter Materie, Vorlesungsmanuskripte des 31. IFF-Ferienkurses, veranstaltet vom 13. bis 24. März 2000*, vol. 3, F4.1–15. Institut für Festkörperforschung der Forschungszentrum Jülich GmbH (2000).

[110] V. Kokoouline, O. Dulieu, R. Kosloff, and F. Masnou-Seeuws. *Mapped Fourier methods for long-range molecules: Application to perturbations in the $Rb_2(0_u^+)$ photoassociation spectrum*. J. Chem. Phys., **110**:9865–9876 (1999).

[111] R. Kosloff. *Time-Dependent Quantum-Mechanical Methods for Molecular Dynamics*. J. Phys. Chem., **92**:2087–2100 (1988).

[112] D. T. Colbert and W. H. Miller. *A novel discrete variable representation for quantum mechanical reactive scattering via the S-matrix Kohn method*. J. Chem. Phys., **96**:1982–1991 (1992).

[113] C. C. Martson and G. G. Ballint-Kurti. *The Fourier grid Hamiltonian method for bound state eigenvalues and eigenfunctions*. J. Chem. Phys., **91**:357–35761 (1989).

[114] M. Monnerville and J. M. Robbe. *Optical potential coupled to discrete variable representation for calculations of quasibound states: Application to the CO($B^1\Sigma^+$ -$D'^1\Sigma^+$) predissociating interaction*. J. Chem. Phys., **101**:7580–7591 (1994).

[115] O. Dulieu and P. S. Julienne. *Coupled channel bound states calculations for alkali dimers using the Fourier grid method*. J. Chem. Phys., **103**:60–66 (1995).

[116] O. Dulieu, R. Kosloff, F. Masnou-Seeuws, and G. Pichler. *Quasibound states in long-range alkali dimers: Grid method calculations*. J. Chem. Phys., **107**:10633–10642 (1997).

[117] F. Gygi. *Adaptive Riemannian Metric for Plane-Wave Electronic-Structure Calculations*. Europhys. Lett., **19**:617–622 (1992).

[118] M. Nest and P. Saalfrank. *Open-system quantum dynamics for gas-surface scattering: Non-linear dissipation and mapped Fourier grid methods*. J. Chem. Phys. (2000). Submitted.

[119] U. Kleinekathöfer and D. J. Tannor. *Extension of the mapped Fourier method to time-dependent problems*. Phys. Rev. E, **60**:4926–4933 (1999).

[120] E. V. Chulkov, I. Sarría, V. M. Silkin, J. M. Pitarke, and P. M. Echenique. *Lifetimes of Image-Potential States on Copper Surfaces*. Phys. Rev. Lett., **80**:4947–4950 (1998).

[121] A. D. Bandrauk, E. Aubanel, and S. Chelkowski. *Molecules in Intense Laser Fields: Applications*. In J. Manz and L. Wöste, eds., *Femtosecond Chemistry*, vol. 2, chap. 25, 731–742. Verlag Chemie (1995).

[122] R. Alicki and K. Lendi. *Quantum Dynamical Semigroups and Applications*. In *Lecture Notes in Physics*, vol. 286. Springer, Berlin (1987).

[123] G. Lindblad. *On the Generators of Quantum Dynamical Semigroups*. Comm. Math. Phys., **48**:119–130 (1976).

[124] V. Gorini, A. Kossakowski, and E. C. G. Sudarshan. *Completely positive dynamical semigroups of N-level systems*. J. Math. Phys., **17**:821–825 (1976).

[125] C. Scheurer and P. Saalfrank. *Hydrogen transfer in vibrationally relaxing benzoic acid dimers: Time-dependent density matrix dynamics and infrared spectra*. J. Chem. Phys., **104**:2869–2882 (1996).

[126] M. Berman, R. Kosloff, and H. Tal-Ezer. *Solution of the time-dependent Liouville-von Neumann equation: Dissipative evolution*. J. Phys. A, **25**:1283–1307 (1992).

[127] G. Alber and P. Zoller. *Laser excitation of electronic wave packets in Rydberg atoms*. Phys. Rep., **199**:231–280 (1991).