MO 20: Quantenkontrolle

Zeit: Donnerstag 16:30–19:00 Raum: Poster C1

MO 20.1 Do 16:30 Poster C1

Control of nuclear spin selective rotation of methyl groups and symmetry adapted quantum dynamics — •Thomas Grohmann and Monika Leibscher — Freie Universität Berlin, Institut für Chemie und Biochemie, Takustr. 3, 14195 Berlin

The control of chemical reaction dynamics is currently intensively studied. However, the influence of the nuclear spin is only little investigated although nuclear spin isomers show different behaviour in their nuclear dynamics [1]. It has been shown, that time-dependent magnetic fields induce molecular rotations in methyl groups [2]. Our aim is to simulate the control of molecular torsion in methyl groups in order to create a molecular motor. Nuclear wavefunctions for methyl groups, obeying the anti-symmetry principle, can be constructed using molecular symmetry groups [3]. We derive the symmetry adapted wavefunctions for explicit model potentials describing nuclear torsion and vibration. By solving the time-dependent Schrödinger equation for the three protons in a time-dependent magnetic field we can show that it is only possible to induce unidirectional rotations if dipolar interactions between the nuclear spins are taken into account.

[1] O. Deeb, M. Leibscher, J. Manz, W. von Muellern and T. Seideman, Chem. Phys. Chem. **8** (2007), 322; T. Grohmann, O. Deeb, and M. Leibscher, Chem. Phys. **338** (2007), 252. [2] S. Clough, A.J. Horsewill, M.R. Johnson, J.H. Sutcliffe and I.B.I. Tomsah, Europhys. Lett. **29** (1995), 169. [3] S. Clough and P.J. McDonald, J. Phys. C **16** (1983), 5753.; K.W.H. Stevens, J. Phys. C **16** (1983), 5765.; D. Haase, private communication

MO 20.2 Do 16:30 Poster C1

Local control theory applied to molecular photoassociation — •Philipp Marquetand and Volker Engel — Institut für Physikalische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Local control theory (LCT) is employed to achieve molecular photoassociation with shaped laser pulses. Within LCT, the control fields are constructed from the response of the system to the perturbation which makes them accessible to a straightforward interpretation. This is shown regarding the ground-state collision of H+F atoms. The objective is to form vibrationally cold associated molecules. Results are presented for s-wave scattering, where the rotational degree of freedom is ignored and also for full scale calculations including rotations, in order to describe more realistic conditions.

MO 20.3 Do 16:30 Poster C1

A New Approach To Optimal Control Theory — •Christian Schwenke[1], Ronnie Kosloff[2] und Christiane P. Koch[1] — [1]Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]Department of Physical Chemistry, Hebrew University, Jerusalem 91904, Israel

Optimal control theory (OCT) was developed to find shaped pulses to control molecular dynamics. Switching the pulse on and off constraints the pulse in time and to create shaped pulses with fs lasers restricts spectral bandwidth. In the iterative approach [1] only one constraint, either in time or in frequency domain, can be imposed. We suggest an optimization scheme which allows for taking into account both constraints by combining the (t,t')-method [2] with OCT. The optimized fields will be found by solving a SCF-like problem.

[1] W. Zhu, J. Botina, H. Rabitz, *Rapid convergent iterative methods for quantum optimal control of population* J. Chem. Phys. **108**, 1953 (1998).

[2] U. Peskin, N. Moiseyev, *The solution of the time-dependent Schrödinger equation by the (t,t')-method: Theory, computational alogorithm and applications* J. Chem. Phys. **99**, 4590 (1993).

MO 20.4 Do 16:30 Poster C1

Experimentelle Realisierung von Laserpulsen im von Neumann Phasenraum — •Alexander Rodenberg[1], Susanne Fechner[2], Frank Dimler[1,2], Tobias Brixner[1,2], David J. Tannor[3] und Gustav Gerber[2] — [1]Institut für Physikalische Chemie, Universität Würzburg, Am Hubland, 97070 Würzburg — [2]Physikalisches Institut, Universität Würzburg, Am Hubland, 97070 Würzburg — [3]Department of Chemical Physics, Weizmann Institute of Science, 76100 Rehovot, Israel

Im Gegensatz zur üblichen Darstellung des elektrischen Feldes im Frequenz- oder im Zeitraum bieten Phasenraumdarstellungen die Möglichkeit, die spektralen und zeitlichen Eigenschaften ultrakurzer Laserpulse simultan und auf intuitive Weise zu erfassen. Vor kurzem haben wir die von Neumann-Repräsentation eingeführt, die im Gegensatz zu den üblicherweise verwendeten eine vollständige Rekonstruktion des elektrischen Feldes bei gleichzeitigem Erhalt der intuitiven Interpretierbarkeit erlaubt. Sie ermöglicht, jeden Laserpuls aus elementaren Subpulsen aufzubauen.

Wir zeigen, wie diese von Neumann-Pulse durch spektrale Amplituden- und Phasenformung experimentell realisiert werden können und diskutieren die hierbei zu beachtenden experimentellen Randbedingungen. Mögliche Anwendungen in der Quantenkontrolle, wie die Vermessung von Fitnesslandschaften oder die Verbesserung vorhandener Lernalgorithmen, werden vorgeschlagen.