

## MO 53 Molecular Quantum Computing

Zeit: Donnerstag 14:00–16:00

Raum: H12

**Fachvortrag**

MO 53.1 Do 14:00 H12

**Efficient implementation of three-qubit quantum gates and experimental demonstration by NMR** — •BJÖRN HEITMANN<sup>1</sup>, NAVIN KHANEJA<sup>2</sup>, HAIDONG YUAN<sup>2</sup>, ANDREAS SPÖRL<sup>1</sup>, THOMAS SCHULTE-HERBRÜGGEN<sup>1</sup>, and STEFFEN J. GLASER<sup>1</sup> — <sup>1</sup>Department Chemie, TU München, Lichtenbergstrasse 4, 85747 Garching, Germany — <sup>2</sup>Division of Applied Sciences, Harvard University, Cambridge, MA 02138, USA

High resolution nuclear magnetic resonance (NMR) currently provides one of the most advanced approaches for the experimental realization of quantum computing concepts. In this talk efficient ways to synthesize quantum gates in three-qubit systems by creating effective interactions between indirectly coupled spins. More specifically, we provide an efficient synthesis of a CNOT gate between two spins that are indirectly coupled via Ising-type couplings to a third spin. Our implementation of the CNOT gate is twice as fast as conventional approaches. This efficient realization of the quantum gate corresponds to computing sub-Riemannian geodesics (1,2) on the unitary group. We provide an experimental realization of the fast indirect CNOT gate on a linear three-spin chain with Ising couplings. The new methods have important applications in quantum information processing and coherent spectroscopy.

References: (1) N. Khaneja, R. W. Brockett, S. J. Glaser, Time Optimal Control in Spin Systems, Phys. Rev. A 63, 03208 2001.

(2) N. Khaneja, S. J. Glaser, R. W. Brockett, Sub-Riemannian Geometry and Time Optimal Control of Three Spin Systems: Quantum Gates and Coherence Transfer, Phys. Rev. A, 65, 032301 2002.

MO 53.2 Do 14:30 H12

**Quantification of Complementarity in Multi-Qubit Systems** —

•XINHUA PENG<sup>1,2</sup>, XIWEN ZHU<sup>2</sup>, DIETER SUTER<sup>1</sup>, JIANGFENG DU<sup>3</sup>, MAILI LIU<sup>2</sup>, and KELIN GAO<sup>2</sup> — <sup>1</sup>Fachbereich Physik, Universität Dortmund, 44221 Dortmund, Germany — <sup>2</sup>Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, P. R. China — <sup>3</sup>Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui 230026, P.R. China

Complementarity was originally introduced as a qualitative concept for the discussion of properties of quantum mechanical objects that are classically incompatible. More recently, complementarity has become a quantitative relation between classically incompatible properties, such as visibility of interference fringes and "which-way" information, but also between purely quantum mechanical properties, such as measures of entanglement. We discuss different complementarity relations for systems of 2-, 3-, or n-qubits. Using nuclear magnetic resonance techniques, we have experimentally verified some of these complementarity relations in a two-qubit system. For three-qubit systems, we also propose an experimental scheme to verify some of the relevant complementarity relations for pure states.

MO 53.3 Do 14:45 H12

**Reducing Decoherence in Large Quantum Registers** — •MARKO LOVRIĆ, DIETER SUTER, and HANS GEORG KROJANSKI — Universität Dortmund, Fachbereich Physik, 44221 Dortmund, Germany

Decoherence appears to be the main limiting factor for the implementation of large (and therefore powerful) quantum computers. While it is generally expected that quantum registers consisting of many qubits will decay faster than smaller ones, the decoherence rates had never been measured for systems with more than 2 qubits. To obtain such data we measure the decay of model quantum registers consisting of up to several thousand nuclear spins. These states can be created by solid-state nuclear magnetic resonance (NMR) techniques. Our results indicate that the decoherence rates increase with the system size, but not as fast as generally expected. For successful operation of a quantum computer it will be essential to reduce decoherence processes. Several approaches have been proposed for decoupling the system from its environment. We have tested several techniques on our model quantum registers and found that it was possible to extend the decoherence time by more than an order of magnitude, independent of the size of the quantum register.

[1] H. G. Krojanski and D. Suter, Phys. Rev. Lett. 93, 090501 (2004)

MO 53.4 Do 15:00 H12

**The role of anharmonicity and coupling in molecular quantum computing** — •CAROLINE GOLLUB, ULRIKE TROPPMANN, and REGINA DE VIVIE-RIEDEL — LMU Department Chemie, Butenandt-Str. 11, 81377 München

Our approach of molecular quantum computing is based on eigenstates of vibrational normal modes of polyatomic molecules encoding the qubits. We analyze the effects of molecular characteristics on the structure of global quantum gates and the complexity of the resulting mechanisms systematically with the goal to judge a molecule's suitability for molecular quantum computing [1]. Decisive properties of molecular vibrations are the anharmonicity and the mode coupling. In a parametrized two-dimensional model system we can tune these characteristical properties and explore their effects on quantum gates. We find that the interplay of the anharmonicity and the coupling is of prime importance and leads to two basic control mechanisms for all systems. The features of the global quantum gates are explained with characteristic transition frequencies, determined by the molecular parameters. The optimal time for the quantum gates and the limits to obtain simple structures are identified. Based on a universal set of optimized quantum gates we realized an efficient quantum fourier transformation [2].

[1] C. Gollub, U. Troppmann and R. de Vivie-Riedel. submitted to NJP

[2] U. Troppmann, C. Gollub and R. de Vivie-Riedel. submitted to NJP

MO 53.5 Do 15:15 H12

**Experimentally feasible quantum gates for MnBr(CO)<sub>5</sub>** — •BRIGITTE KORFF<sup>1</sup>, ULRIKE TROPPMANN<sup>2</sup>, KARL L. KOMPA<sup>1</sup>, and REGINA DE VIVIE-RIEDEL<sup>2</sup> — <sup>1</sup>MPI für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching — <sup>2</sup>LMU München, Department Chemie, Butenandt-Str. 11, 81377 München

In our concept for quantum computing qubits are encoded in vibrational normal modes of polyatomic molecules. Quantum gates are implemented by shaped femtosecond laser pulses. We adopt this concept to Manganese-pentacarbonyl-bromide (MnBr(CO)<sub>5</sub>) [1] a promising candidate in the mid-IR frequency range to connect theory and experiment. The 2D ab initio potential energy surface (PES) and the associated dipole vector surfaces spanned by the two strongest IR active modes are computed with DFT. Allowance for environmental effects makes the model flexible for variable experimental conditions. From the PES the vibrational eigenstates representing the qubit system are calculated. Laser pulses are optimized by multi target optimal control theory (MTOCT) to form a set of elementary global quantum gates. For all of them simply structured pulses with low pulse energies around 1 μJ and switching efficiencies above 99% could be obtained. Exemplarily for the CNOT gate we investigated the possible transfer to the experiment based on the mask function for pulse shaping in the frequency regime as well as decomposition into a train of gaussian subpulses.

[1] B. Korff et al, J. Chem. Phys. 123 (2005) 23xxxx

**Fachvortrag**

MO 53.6 Do 15:30 H12

**Realization of Molecular Logic Gates by Femtosecond Multi-Photon Interaction** — •A. MATERNY, J. KONRADI, A.V. SCARIA und A.K. SINGH — International University Bremen, Bremen

Um ein logisches Gatter mit Hilfe eines Moleküls zu verwirklichen, können Mehrphotonenwechselwirkungen genutzt werden. Die Ordnung des nichtlinearen Prozesses entscheidet über die Komplexität, die Pulsdauer und molekulodynamische Parameter über die Geschwindigkeit des "Bausteins". In einer früheren Arbeit haben wir die Möglichkeit einer stimulierten Raman-Anregung (zwei Pulse) mit anschließender kohärenter anti-Stokescher Raman Streuung (CARS, Vierphotonenprozess) zur Verwirklichung eines Dreibit-Gatters ("Toffoli Gatter") diskutiert [1]. Hierbei werden Schwingungsmoden des Moleküls in Abhängigkeit von den beteiligten Laserpulsen genutzt und durch geeignete Kombinationen alle möglichen Gatterschaltungen (UND, ODER, usw.) verwirklicht. Unsere neuesten Arbeiten weisen auf eine Möglichkeit, diese logischen Gatter zu optimieren. Mit Hilfe der selbstlernenden Optimierungstechnik, können wir zwischen verschiedenen molekularen Schwingungsmoden hin- und herschalten [2]. In einer fs-CARS-Wechselwirkung bestimmt der elektronisch resonante oder nichtresonante Anregungsschritt (zwei Pulse, einer optimal geformt), welche spektrale Verteilung im Signal durch den Abfrageschritt erzeugt werden kann.

- [1] A. N. Naumov, A. Materny, W. Kiefer, M. Motzkus, and A. M. Zheltikov, *Laser Phys.* **11**, 1319, (2001).  
[2] J. Konradi, A.K. Singh, A. V. Scaria, and A. Materny, *J. Raman Spectrosc.*, in press (2006).