CPP 2: Tutorial: Physics of NMR - Physics with NMR

Time: Sunday 16:00–18:30 Location: H3

Tutorial CPP 2.1 Sun 16:00 H3

Spins as Qubits — •Dieter Suter — Fakultät Physik, TU Dortmund

Processing of digital information has progressed at an enormous speed over the last decades and thus become an indispensable resource. Still, for some computational problems, no efficient algorithms are known for today's computers. For some of these problems, an exponential speedup is possible if the computers operate according to Schrödinger's equation, processing the information by unitary transformations. Nuclear spins were the first physical systems used to implement quantum algorithms; in the meantime, several other systems have become available for quantum information processing, all drawing directly from the techniques that NMR has developed for accurately controlling the dynamics of quantum mechanical systems. We will discuss some demonstration experiments that use magnetic resonance techniques to process quantum information stored in nuclear and electronic spins. Since today's quantum computers are based on a small number of qubits, their computational power is quite limited. To make them more powerful, it will be necessary to increase the number of qubits. Many concepts have been proposed that may eventually unlock this potential, some of them based on electronic and nuclear spins.

Literature: J. Stolze and D. Suter, *Quantum Computing: A Short Course from Theory to Experiment*, Wiley-VCH, Berlin, 2nd edition (2008).

short session break

Tutorial CPP 2.2 Sun 17:00 H3

Kernspin-Gitter-Relaxation: Grundlagen, Beispiele, Instrumentierung — •Franz Fujara — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt

Im ersten Teil des Vortrags werde ich einige grundlegende Begriffe (Ratengleichungen, Wechselwirkungs-Hamiltonian, Übergangswahrscheinlichkeiten) der elementaren semiklassischen Relaxationstheorie einführen, womit dann Phänomene wie die Relaxationsrate, die Spindiffusion, die Spintemperatur und Fragen der (Nicht)ergodizität diskutiert werden können. Sodann möchte ich instruktive Resultate der traditionellen (Festfrequenz-)Relaxometrie vorstellen, die das Potenzial und die Limitierungen des Verfahrens verdeutlichen. Der letzte Teil des Vortrages behandelt moderne Field-Cycling (FC) Relaxometrieverfahren, sowohl elektronische als auch mechanische. Anhand aktueller experimenteller Beispiele soll ausgeführt werden, dass die FC-Relaxometrie als breitbandiges dynamisches Suszeptibilitätsverfahren betrachtet werden kann, welches mit erheblichem Gewinn gemeinsam mit der Messung anderer dynamischer Suszeptibilitäten, z. B. der dielektrischen Relaxation oder der dynamischen Lichtstreuung, eingesetzt werden kann.

Tutorial CPP 2.3 Sun 17:45 H3

NMR at High Pressures and High Fields — •Hans Robert Kalbitzer — Institute of Biophysics and Physical Biochemistry, University of Regensburg, D-93040 Regensburg, Germany

The two main methods for biomolecular structure determination are X-ray crystallography and NMR spectroscopy. The major advantage of the former is that virtually no size limit exists for the investigated macromolecules. Yet, only well crystallizeable systems can be analyzed preventing the investigation of for example transient complexes. NMR has the benefit that analysis can be performed in solution under nearly physiological conditions and dynamics can be studied in detail. High pressure NMR has developed in the last decade to a valuable tool for studying biophysical properties of proteins. Static pressure up to 400 MPa is applied to the sample located inside the high-field NMR spectrometer. The pressure is transferred to the sample cell via a pressurizing fluid and can be changed during the experiments. Besides an anisotropic compression of the protein, the most important feature of high pressure NMR spectroscopy is that conformational equilibria can be shifted reversibly, allowing the detection and structural characterization of excited states that are only weakly populated at ambient pressure. Time-dependent non-equilibrium states can be detected by pressure-jump NMR spectroscopy where the pressure is changed repeatedly by approximately 100 MPa in a time scale of 30 ms inside the NMR spectrometer. The pressure response is correlated to NMR parameters by introducing the pressure jumps in a complex pulse sequence (pressure correlation spectroscopy).