NMR: from new mathematical methods to materials science

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Solid state NMR is a vivid field of research both from theoretical and experimental points of view. After a brief presentation of the experimental topics currently developed at the LCMCP, we will focus on a new mathematical theory named Path-Sum (Giscard, 2012). For any finite square matrix **A**, it is demonstrated that each entry of $\mathbf{A}^m$ (A to the power m) is obtained analytically by a finite resummation on simple cycles and paths (primes) of the finite graph associated to **A**. This fundamental result is analogous to the fundamental theorem of arithmetic (involving integers and prime numbers). Path-Sum is also applicable to the exact calculation of the ordered exponential of **A**, in other words to the NMR evolution operator **U** — namely ***the*** target in spin dynamics.

We will illustrate these new concepts by taking explicit examples: circularly polarized excitation, linearly polarized excitation and Bloch-Siegert effect, static and MAS (magic angle spinning) dipolar hamiltonian in the case of N spins. Spin diffusion pathways will be illustrated by large clusters containing tens of protons.

Reference

P.-L. Giscard, S.J. Thwaite, D. Jaksch, "Walk-sums, continued fractions and unique factorisation on digraphs", arXiv:1202.5523 (**2012**).