New Strategies for Quantum Control of Nuclear Spins in Molecules

Johannes K. Krondorfer, Matthias Diez and Andreas W. Hauser

Two recently proposed strategies for the manipulation of nuclear spins are presented and evaluated on a theoretical level via a combination of quantum simulation and electronic structure theory.[1,2,3] Both suggestions attempt to overcome the problem of addressing specific, single nuclear spins, a problem intrinsic to any method involving magnetic fields.

The first method identifies the vibrational excitation of pseudorotational motions in suitable, highly symmetric molecules as a possible way to generate localized magnetic fields. With the help of these local magnetic fields, even spin states of identical atoms within the same molecule might become individually addressable. The second method exploits the nuclear electric quadrupole moment of non-spherical nuclei to access nuclear spin states through time-dependent electric fields.

Both methods have in common, that they aim for a link between individual nuclear spin manipulation and well established technologies such as microelectronics and quantum optics. On the long run, by introducing pulsed lasers in the optical or IR regime as a tool for spin control, the long coherence times of the nuclear spin degrees of freedom might become accessible via known and proven technology standards.

(1) Wilhelmer, R.; Diez, M.; Krondorfer, J. K.; Hauser, A. W. Molecular Pseudorotation in Phthalocyanines as a Tool for Magnetic Field Control at the Nanoscale. *J. Am. Chem. Soc.* **2024**, *146* (21), 14620–14632. https://doi.org/10.1021/jacs.4c01915.

(2) Krondorfer, J. K.; Diez, M.; Hauser, A. W. Optical Nuclear Electric Resonance in LiNa: Selective Addressing of Nuclear Spins through Pulsed Lasers. *Phys. Scr.* **2024**, No. 99, 075307. https://doi.org/10.1088/1402-4896/ad52fe.

(3) Krondorfer, J. K.; Hauser, A. W. Nuclear Electric Resonance for Spatially Resolved Spin Control via Pulsed Optical Excitation in the UV-Visible Spectrum. *Phys. Rev. A* **2023**, *108*, 053110. https://doi.org/10.1103/physreva.108.053110.