MOLECULAR QUBITS

Quantum information leakage

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Qubits — the fundamental units of quantum computers — are based on particles, such as electrons and nuclei, that can assume two spin states. Quantum computing relies on the coherent phase relationship between the quantum states associated with the spin energy levels. However, interaction of the system with the external environment leads to decoherence and compromises the quality of information processing. Coherence is not completely lost, though. Writing in the *Journal of Physical Chemistry Letters*, Jia Chen, Xiao-Guang Zhang and colleagues report that the residual coherence can be calculated to provide useful information on the decoherence process.

Magnetic molecules have been identified as very promising platforms for the control of the electron spins as their quantum properties can be tuned by changing the molecular structure and its interaction with the surroundings. Although molecular spin qubits have shown prolonged coherence times, they are still not completely immune to decoherence. The interaction between electron and nuclear spins through what is known as hyperfine coupling is the principal

cause for decoherence in molecular systems at low temperatures.

Decoherence occurs through the longitudinal and transverse spin relaxation mechanisms. “During the transverse relaxation process, the system — electron spin in this case — prepared in a pure quantum state evolves into a mixed state because of its interactions with the environment — in this case, nuclear spins. In essence, quantum information leaks out into the environment,” explains Chen. Longitudinal relaxation is considered a thermal process and, at low temperature, occurs over a longer time with respect to the transverse relaxation.

Danna Freedman and co-workers from Northwestern University had previously studied the transverse relaxation time in vanadyl complexes $(\text{Ph}_4\text{P})_2[\text{VO}(\text{C}_3\text{H}_6\text{S}_2)_2]$, $(\text{Ph}_4\text{P})_2[\text{VO}(\text{C}_5\text{H}_6\text{S}_4)_2]$, $(\text{Ph}_4\text{P})_2[\text{VO}(\text{C}_7\text{H}_6\text{S}_6)_2]$ and $(\text{Ph}_4\text{P})_2[\text{VO}(\text{C}_9\text{H}_6\text{S}_8)_2]$ using electron paramagnetic resonance. They looked at the response of the transverse relaxation to the increasing distance between the vanadium and spin active hydrogens.

“Our work is inspired by the experimental results from

Dr Freedman’s group, which revealed that stronger inter-molecular hyperfine couplings can lead to longer coherence time. Our study aims to explain this counter-intuitive observation. We would also like to formulate a suitable theoretical framework to help connect molecular structures to decoherence processes in molecular qubits,” says Chen.

The group led by Zhang performed density functional theory calculations of the hyperfine coupling tensors between electron and nuclear spins of vanadium and the distal hydrogen atoms in the same vanadyl complexes investigated by Freedman and co-workers. They found that, for single molecules, decoherence is often incomplete, with the residual coherence being greater for smaller molecules, which consequently have longer coherence times than larger vanadyl complexes.

This result supports the idea that nuclear diffusion is partially suppressed when nuclear and electron spins are in close proximity.

“One implication of this result is that nuclear spins are not always bad for coherence and we need to understand the effect of nuclear spins better,” remarks Chen. “Because residual coherence can be calculated from first-principles calculations, we hope that this new concept can be helpful in the design of molecular qubits,” he concludes.

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ORIGINAL ARTICLE Chen, J. et al. Decoherence in molecular electron spin qubits: insights from quantum many-body simulations. *J. Phys. Chem. Lett.* **11**, 2074–2078 (2020)

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