OPTIMIZING SURFACE-BASED QUANTUM ARCHITECTURES WITH QUANTUM OPTIMAL CONTROL THEORY

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Optimal Control Theory (QOCT) provides a powerful framework for steering quantum systems with high precision—an essential capability for fast and accurate quantum operations. This talk explores QOCT's role in advancing surface-based quantum platforms: nuclear-spin qudits in lanthanide single-molecule magnets (SMMs), holmium single-atom magnets (SAM) on surfaces whose nuclear spins can serve as qudits with an extraordinarily small Landau–Zener gap, and electronic-spin qubits controlled by electron spin resonance scanning tunneling microscopy (ESR-STM).

In SMMs such as $TbPc_2$, nuclear spin manifolds (e.g., I = 3/2) offer multi-level qudits that enable compact quantum gate implementations. Experiments by Godfrin *et al.*[1,2] have demonstrated quantum gate operations and even Grover's algorithm using electrically driven nuclear spins. However, scaling to higher-dimensional qudits introduces more decoherence channels, potentially offsetting their advantages. Recent theoretical studies have clarified when qudits can outperform equivalent multiqubit schemes, provided operations are fast and high-fidelity[3,4]. Here, QOCT—combined with models of nuclear spin-electric field coupling—offers a way to tailor control fields and preserve this performance edge. Moreover, the same theoretical framework can be applied to Ho SAM-based nuclear spin qudits that can be controlled via ESR-STM.

Meanwhile, ESR-STM also allows for atomic-scale manipulation of individual electronic spins, with Wang *et al.*[5] achieving coherent single-qubit and small-scale multiqubit gates (CNOT and CCNOT). Yet, crucial milestones—like scalable entanglement and robust n-qubit operations—remain unmet[6]. To address this, we develop realistic models of spin dynamics using open quantum system simulations and apply QOCT to design optimal, experimentally viable gate protocols.

In both cases, QOCT serves as a bridge between physical modeling and experimental feasibility, enabling precise control under realistic constraints. By tackling platform-specific decoherence and control challenges, this work supports the development of scalable, surface-based quantum information technologies.

References

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