

# Digital Quantum Simulation of Spin Transport

## Scientific Achievement

QSC researchers led by Purdue University have demonstrated the first digital quantum simulations of the current autocorrelation function for 1-D Heisenberg spin chains. Their results create a programmable application for simulating quantum spin transport of model materials in the ballistic, diffusive and superdiffusive regimes.

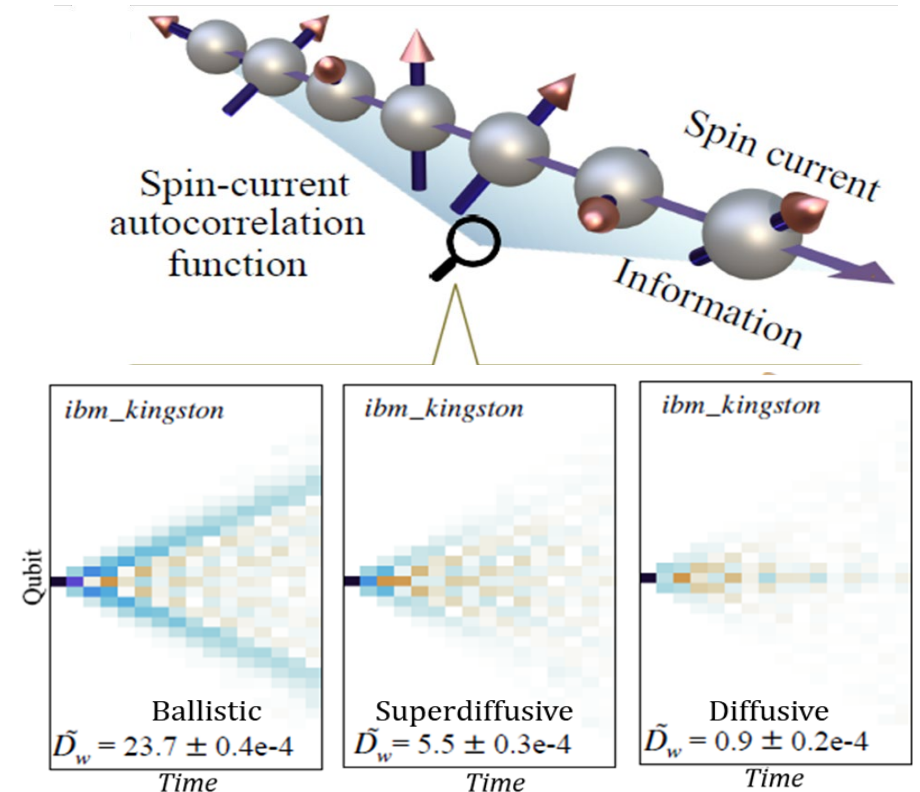
## Significance and Impact

Spin transport measurements are a prominent characterization method in condensed matter physics. These results demonstrate how to simulate spin transport using a quantum computer as a new pathway for understanding complex quantum materials. The results also serve as an important step towards simulating more complex thermal transport measurements that can be used to interrogate future 2-D spin lattices.

## Technical Approach

- The collaborative work was led by QSC members at Purdue University and IBM with collaborators from University of Illinois Urbana Champagne.
- The simulation of a 40-qubit model of a 1D XXZ Hamiltonian was run on the *ibm\_kingston* quantum computer using 2<sup>nd</sup> order Suzuki–Trotter time evolution.
- Simulation results were compared directly to materials samples,  $\text{KCuF}_3$  and  $\text{YbAlO}_3$ , using Spin-Seebeck and inelastic neutron scattering as well as numerical validation.

Yi-Ting. Lee, Bibek Pokharel, Jeffrey Cohn, Andre Schleife, Arnab Banerjee, “Digital Quantum Simulation of Spin Transport”, Physical Review Letters 136, 050603 (2025). DOI: 10.1103/mx9k-kdlj



(top) When a central spin is perturbed, information spreads via propagating quantum fluctuations. (bottom) Different spin transport behaviors are seen in a 40-qubit simulation of the 1D Heisenberg model: ballistic (left), superdiffusive (center), and diffusive (right) regimes are characterized by the rate of spin spreading with KPZ exponents and uniform fluctuations in all length-scales.

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- **NQISRC Intellectual Role:** *Lead*
- **NQISRC Funding Role:** *Majority*
- **Explanation of Funding Institution Contributions**
  - DOE Office of Science, Quantum Science Center
  - IBM Illinois Discovery Accelerator Institute
  - University of Illinois Urbana Campaign Scholarship