Quantum Spin Microscopy's Emerging Methods, Roadmaps, and Enterprises

John A. Sidles, Joseph L. Garbini, Jonathan P. Jacky, and Rico A. R. Picone

Quantum Systems Engineering Laboratory, University of Washington, Seattle, WA, USA

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Achieving three-dimensional, in-depth, atomic-resolution biological microscopy of undenatured specimens is one of the oldest dreams of science. Recently an IBM team led by Dan Rugar and John Mamin has taken us substantially closer to this goal [1] using magnetic resonance force microscopy (MRFM) to obtain three-dimensional images of tobacco mosaic viruses having voxel resolution down to $\sim 4\,\mathrm{nm}$. A 1946 letter from John von Neumann to Norbert Wiener [2] invites Wiener to consider whether comprehensive atomic-resolution biological microscopy might be achieved "by developments of which we can already foresee the character, the caliber, and the duration. And are the latter two not excessive and impractical?" Obtaining reliable answers to von Neumann's question is the overall objective of this work.

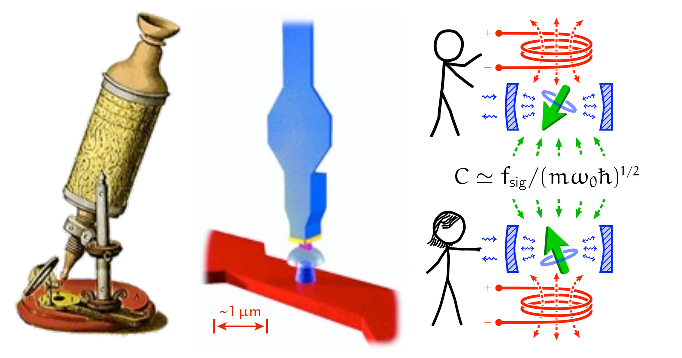

Figure 1 Magnetic resonance microscopes can be viewed as communication channels between the sample and microscope. Present microscopes are far from quantum limits [3].

Emerging Methods Our practical focus is the development of numerical algorithms for the end-to-end simulation of atomic-resolution quantum spin microscopy [3], with emphasis upon polarization transport processes. Here "end-to-end" means an integrated simulation of all the dynamical elements of a quantum spin microscope, from macroscopic elements like sample positioners, to mesoscopic elements like force microscope cantilevers, to fully quantum elements, like the individual spins in supramolecular structures. In brief, the simulation strategy is to transcribe Hilbert-space descriptions of quantum dynamics into the geometric language of symplectic flows and Lindbladian stochastic processes [4, 5].

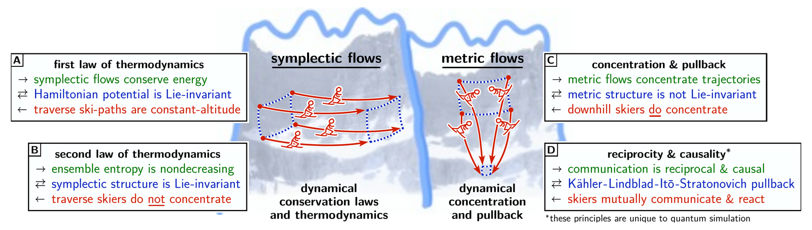

Figure 2 Dynamical processes in spin microscopy are naturally described in terms of symplectic flows (**A–B**) that respect thermodynamical laws, and metric flows (**C–D**) that describe measurement, control, and noise processes. In consequence of compressive Lindbladian dynamics, numerical trajectory integration is efficient even for systems of hundreds of spins [5].

Emerging Roadmaps and Enterprises As large-scale quantum simulation methods become more efficient, quantum systems engineering methods become more practical; in consequence the present decade is effectively a "Sputnik Moment" for magnetic resonance research and enterprise that is witnessing a "Cambrian Explosion" of diverse experimental methods and theoretical ideas. Our present theoretical and experimental investigations are exploring the physics of polarization transport processes in large magnetic gradients, with a view toward achieving by dynamical nuclear spin polarization an MRFM signal strength sufficient for imaging with $(0.5\,\mathrm{nm})^3$ voxel resolution, sufficient for the direct imaging of (for example) the changes in chromatin architecture that are associated to cell differentiation in regenerative healing processes.

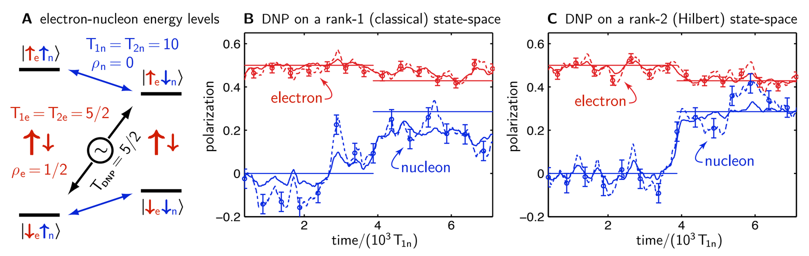

Figure 3 The large magnetic gradients of spin microscopes are a new environment for polarization transport. Novel (and potentially practical) mechanisms for dynamical spin polarization are associated to these gradients [5].

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