

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

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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 ~ 4 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.

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 microscopic 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].

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 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.

Acknowledgements This work is dedicated to the families of the *Ceremony in Honor of Wounded Marines*, 12 May 2006, Marine Corps Barracks, Washington, DC. This research is supported by the Army Research Office (ARO) under MURI program # W911NF-05-1-0403. Presented as poster #PA-15, 52nd ENC, April 10–15 2011, Asilomar CA.

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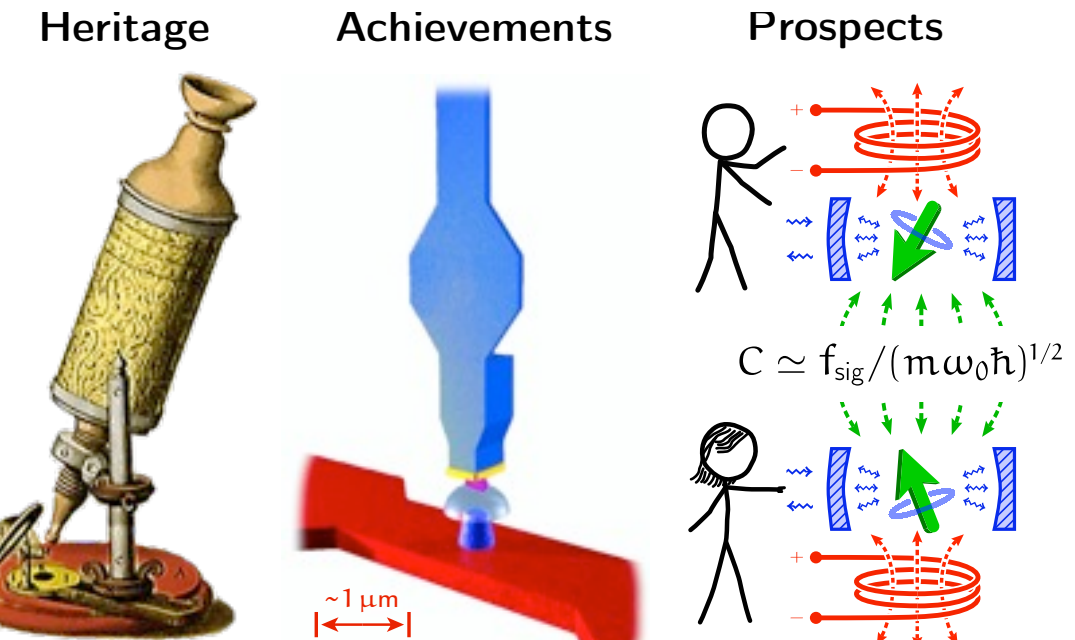


Figure 1 Magnetic resonance microscopes can be viewed as communication channels between the sample and microscope. Present microscopes are far from quantum limits [3].

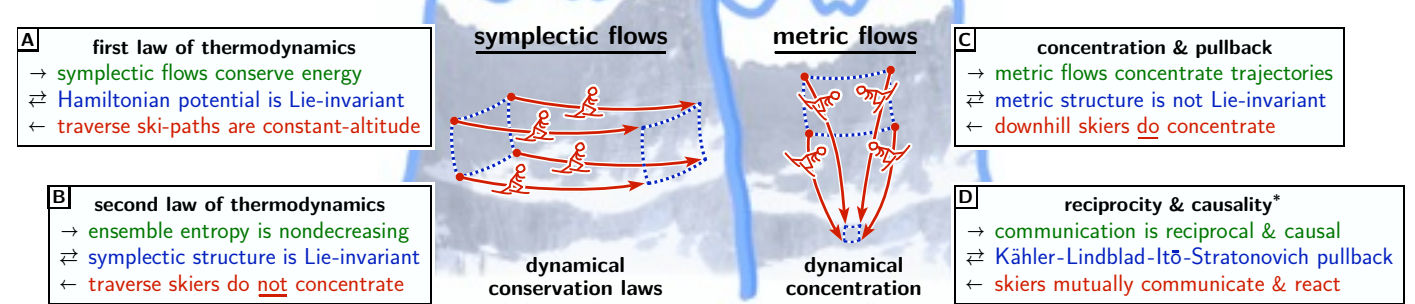


Figure 2 Dynamical processes in spin microscopy are naturally described in terms of symplectic flows (A–B) that respect thermodynamical laws, and metric flows (C–D) that describe measurement, control, and noise processes. In consequence of compressive Lindbladian dynamics, numerical trajectory integration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

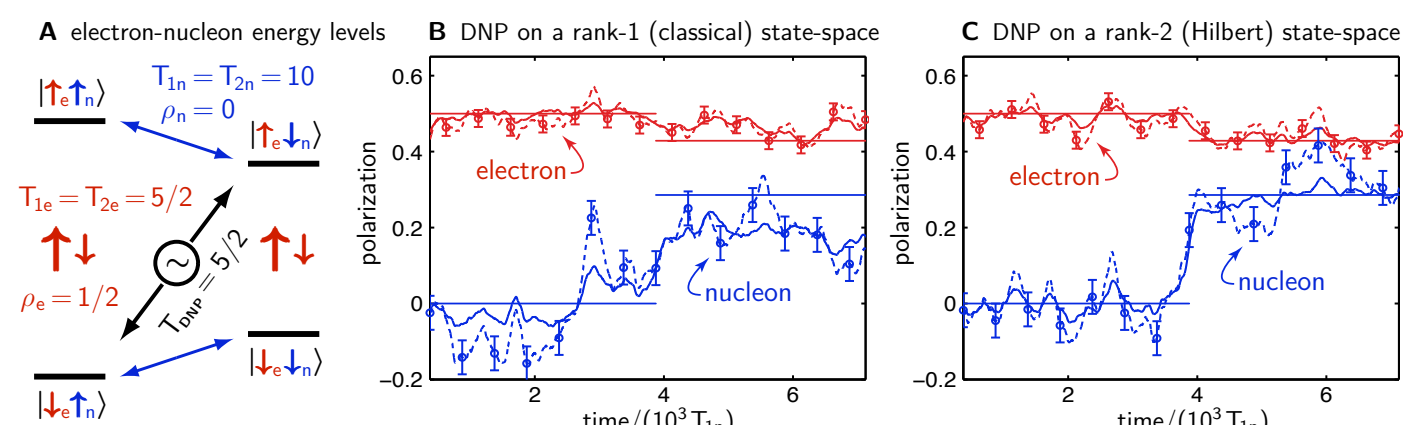
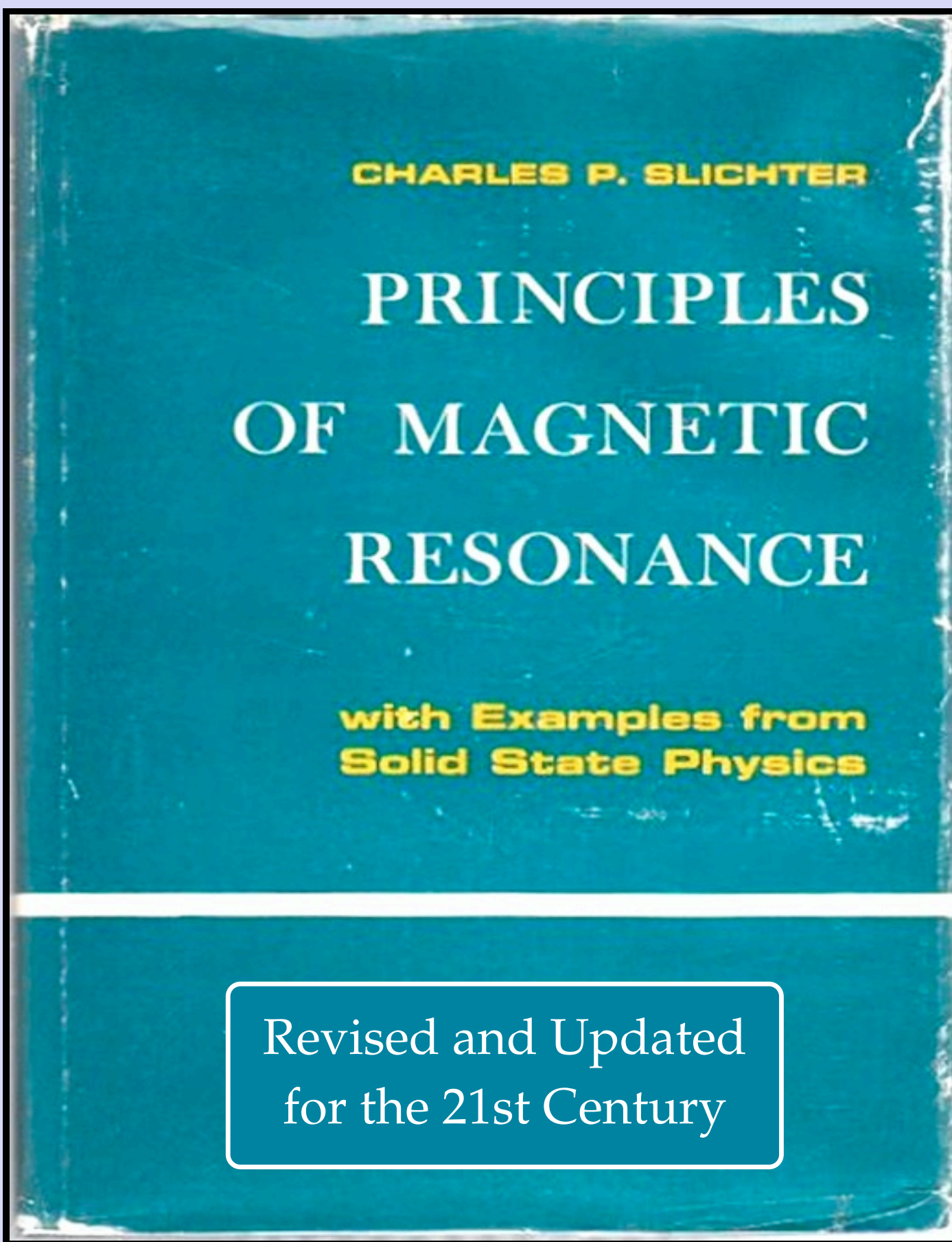


Figure 3 The large magnetic gradients of spin microscopes are a new environment for polarization transport. Novel (and potentially practical) mechanisms for dynamical spin polarization are associated to these gradients [5].



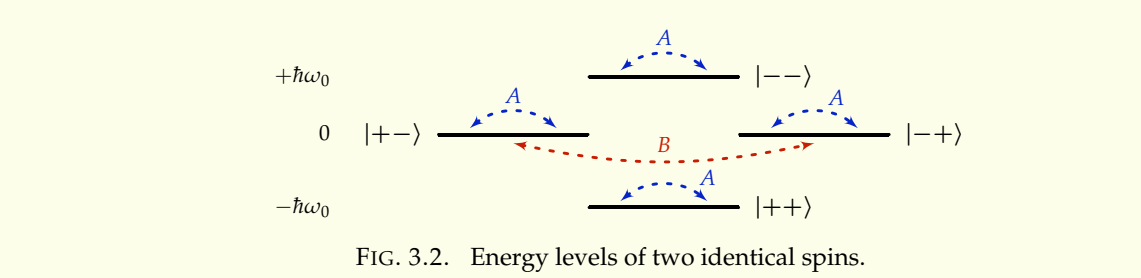
Revised and Updated for the 21st Century

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that an operator and its symbol function each determine the other. In geometric dynamics, the (complex) functions $\langle \psi | \cdot | \psi \rangle$ are a coordinate atlas on the Hilbert state-space and the (real) functions $\langle \psi | \cdot | \psi \rangle$ are dynamical potentials. Soon we will demonstrate (see Theorem 1) that specifying quantum dynamics in terms of symbol functions is substantial practical advantages.

As we have remarked, $(\gamma_1 \gamma_2 \hbar^2)^{1/2}$ corresponds to the interaction of a nuclear magnet with a field of about 1 gauss, whereas the Zeeman Hamiltonian $H_Z = -\gamma_1 \hbar \omega_1 I_1 - \gamma_2 \hbar \omega_2 I_2$ corresponds to an interaction with a field of 10^4 gauss. It is therefore appropriate to solve the Zeeman problem first and then treat the dipole term as a small perturbation. (Actually, for two spins of $\frac{1}{2}$, an exact solution is possible.)

We shall diagram the appropriate matrix elements and energy levels in Fig. 3.2.



It is convenient to denote a state in which $m_1 = \pm \frac{1}{2}$, $m_2 = \pm \frac{1}{2}$ by the notation $| \pm \pm \rangle$. The two states $| + - \rangle$ and $| - + \rangle$ are degenerate, and both have $E_Z > 0$. The states $| + + \rangle$ and $| - - \rangle$ have respectively $-E_Z$ and $+E_Z$, where $E_Z = \gamma \hbar \omega$ as usual. We first inquire into what parts of states are connected by the various transitions. A convenient notation for the term A , which is proportional to $\langle \psi | A | \psi \rangle$, is clearly convenient. It connects $| m_1 m_2 \rangle$ with $| m_1' m_2' \rangle$. On the other hand, B , which is proportional to $\langle \psi | B | \psi \rangle$, only connects $| m_1 m_2 \rangle$ to states $| m_1' m_2' \rangle$ in which $m_1' = m_1$ or $m_2' = m_2$. A customary parlance is to say that B simultaneously flips one spin up and the other down. B therefore can join only the states $| + - \rangle$ and $| - + \rangle$.

We can express these same physical ideas more formally via operator algebra. The following commutation relations are readily verified:

$$[A_1, I_2] = 0 \quad \text{and} \quad [A_2, I_1] = 0$$
$$[B_1, I_2] \neq 0 \quad \text{and} \quad [B_2, I_1] \neq 0$$
$$[B_1, I_1] = \hbar \omega_1 I_1 \quad \text{and} \quad [B_2, I_2] = \hbar \omega_2 I_2$$

which is to say, the A interaction conserves z -axis polarization of spin-species 1 and 2 separately, while the B interaction conserves only their sum.

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Definitions and synopsis. Let \mathcal{H}_k be a Hilbert space of vectors ψ that is spanned by a preferred basis that is given as an orthonormal set of n -factor tensor products (in physical terms, such a basis is variously called an *n*-particle, *n*-spin, or *n*-qudit basis). Allow the component vectors of the n -factor product to have various dimensions (in physical terms, allow the individual particles to carry various quantum numbers). Let ψ be any linear Hilbert operator that when given in the n -factor basis acts solely upon one particle (for example, 1 can mislabel one single-particle quantum numbers and associate to it the bilinear symbol function $\langle \psi | \psi \rangle$). Let \mathcal{H}_k be any n -factor Hilbert operator that when given in the n -factor basis acts solely upon one particle (for example, 1 can mislabel one single-particle quantum numbers and associate to it the bilinear symbol function $\langle \psi | \psi \rangle$). 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