## 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

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

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

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 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 Figure 1 Magnetic resonance microscopes can be viewed as 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 endto-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 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

**Emerging Roadmaps and Enterprises** As largescale 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 experi-

Spin microscopy's heritage, achievements, and prospects

Quantum Systems Engineering Laboratory, School of Medicine, and College of Engineering, University of Washington, Seattle,

which you Neumann discusses, at con-

the character, the caliber, and the duraShannon's waterfilling integral (equation in 24 h. Together with inevitable real-

32 in ref. 4) for  $S_f$  and  $S_g$  varied with

Inserting these IBM device parame-

main focus of this commentary. Von

perhaps would be pleased that the

methods of their colleague Enrico

design and systems engineering (5).

this Fermi calculation starting point.

that a stronger capacity bound is ob-

Fermi are now regarded as essential to

Multiple paths of inquiry depart from

Communication theorists will recognize

tained by specifying  $S_f$  and  $S_q$  individu-

ally, rather than constraining only their

bits/s. This means that the IBM team

The coefficient 0.476 is the extremum of lent to transmitting a 90-kB image file 1E-mail: sidles@u.washington.edu

product  $S_f$   $S_g$  as in Eq. 1. The resulting

commentary's focus, and we seek to ters into Eq. 1, we compute a capacity

describe paths by which mathematicians, bound of  $C \leq 40$  bits/s. This figure-of-

ng, frequency  $\omega_0/(2\pi) \simeq 2.9$  kHz, force noise nearly optimally. Good.

noise  $S_f^{1/2} \approx 10 \text{ aN/VHz}$  (one-sided), and Imaging researchers will appreciate

measurement noise  $S_n^{1/2} \approx 1.0 \text{ pm/VHz}$ . that 8.5 bits/s is painfully slow, equiva-

of the IBM Research Division (Center) extend and strengthen this heritage. These achievements lead us

conceive of microscopy as sample spins (Alice, at lower right) transmitting information to observers (Bob,

at upper right). With continued advances in nanotechnology, materials science, quantum informatio

science, and many other disciplines—advances that in aggregate are transforming present conceptions o

merit, and elaborations of it, will be the stand ready to be applied, including sig

Neumann and Wiener would recognize initio information into modulation and

this approach as a Fermi calculation, and deconvolution algorithms, and (very re-

world inefficiencies, this explains the

and an array of remediating technique

nal multiplexing, incorporation of ab

It is good to acquire data faster, so let

us now consider paths for boosting the

Quantum information researchers wi

recognize that the noise product  $S_fS_q$  is

ion 6.7 in ref. 6), which is called the

standard quantum limit (SQL). Eq. 1

Author contributions: J.A.S. wrote the paper.

PNAS | February 24, 2009 | vol. 106 | no. 8 | 2477–2478

then implies the *test-mass capacity bound* 

See companion article on page 1313 in issue 5 of volume

 $C \le 0.476 \times f_{\text{sig}}/(m\omega_0 \hbar)^{1/2}$ . [2]

raw channel capacity of Eq. 1.

piological microscopy of unde

natured specimens is one of

oldest dreams of science, and for

ood reason: it unites the thrilling pros-

itiers with cutting-edge technical

challenges from every domain of mathe-

In a recent issue of PNAS, a team

om IBM Research led by Dan Rug

and John Mamin has taken us a giant

tic resonance force microscopy

(MRFM) to obtain 3-dimensional im-

ages of tobacco mosaic viruses having

tel resolution down to ≈4 nm. Ou

be modeled on a 1946 letter from John

on Neumann to Norbert Wiener (2), in

siderable length, both the practical prob

lem of achieving atomic-resolution bio-

nann's letter invites Wiener to consider

whether atomic-resolution biological mi-

croscopy might be achieved "by develop

tion. And are the latter two not exces-

scientists, and engineers—of almost ev-

ery discipline—can contribute to, or

penefit from, this centuries-old quest.

by Alice so as to create a signal force

We ask the natural question, how fast

can Alice transmit information to Bob?

This rate, called the *channel capacity*, is

f(t) that is observed by Bob (Fig. 1)

 $C \le 0.476 \times f_{\text{sig}} / (m^2 \omega_0^2 S_f S_q)^{1/4}.$ 

as follows: Alice's root-mean-square

force signal is  $f_{\text{sig}} \simeq 10$  aN, Bob's

The meaning of these parameters and

their values in the IBM experiments are

MRFM cantilever has mass  $m \approx 0.26$ 

www.pnas.org/cgi/doi/10.1073/pnas.0813322106

1949 Capacity Theorem as

We begin by conceiving of spin mi-

ard sample spins as being modulated

We adopt von Neumann's question as

ments of which we can already foresec

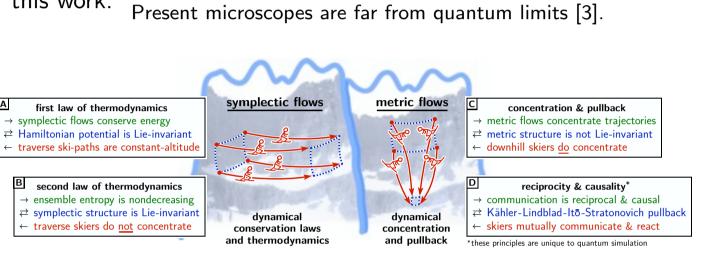
logical microscopy and the potential

mments on the IBM experiment will

step closer to this goal (1) by using mag-

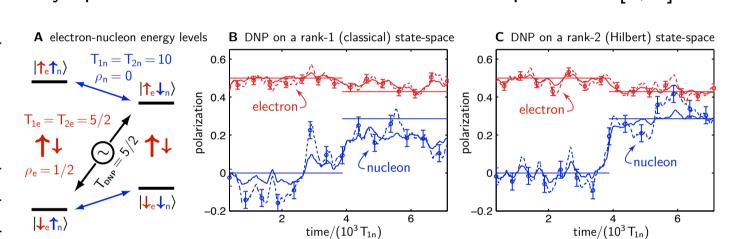
pect of opening vast new scientific

communication channels between the sample and microscope.



scopic elements like sample positioners, to meso- 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].

of quantum dynamics into the geometric language of symplectic flows and Lindbladian stochastic processes [4, 5].



mental methods and theoretical ideas. Our present Figure 3 The large magnetic gradients of spin microscopes are a new environtheoretical and experimental investigations are ex- ment for polarization transport. Novel (and potentially practical) mechanisms ploring the physics of polarization transport pro-

periment (8), the first detection of sta-imaging (13–16) that has greatly ex-

irst detection of gradient suppression of and opportunities of quantum spin

on) spin (11), and now the first high-culation (Eq. 3) illuminates multiple

Let us consider one final Fermi calcuple: the obvious parameter to improve

some of the paths that lie ahead. We Ought we to begin conceiving of spin

Braginsky VR, Khalili FY (1992) Quantum Measurement spin detection by magnetic resonance force micros-

lation, with a view toward illuminating in Eq. 3 is the quantum number  $i_{\rm B}$ .

tection and imaging of a single (elec-

resolution MRFM biological images (1).

2478 | www.pnas.org/cgi/doi/10.1073/pnas.0813322106

istical polarization by MRFM (9), the panded our conception of the challenges tations of our present tools. We de-

Now for the third time our Fermi cal-

008) Nanoscale magnetic resonance imaging. Proc detection of magnetic resonance. Nature 360:563– with a diamond single-spin sensor. Appl Phys Lett

mp Appl Math 52:506–512.

oke R (1665) Micrographia (Royal Society, London).

innon C (1949) Communication in the presence of 10. Budakian R, Mamin HJ, Rugar D (2004) Suppression of 12. Maze JR, et al. (2008) Nanoscale magnetic sensing with

1. Rugar D, Budakian R, Mamin HJ, Chui BW (2004) Single 16. Taylor JM, et al. (2008) High-sensitivity diamond r

noise. Proc Inst Radio Eng 37:10–21. spin diffusion near a micron-size ferromagnet. Phys
Magrab EB (1997) Integrated Product and Process Design Rev Lett 92:037205. an individual electronic spin in diamond. Nature 455:644–647.

Sidles IA. Garhini IL. Drobny GP (1992) The theory of 12. Sidles JA, et al. (2008) Practical recipes for the model 17. Romalis M (2008) Applied physics: Virtues of diamond

applications to molecular imaging. Rev Sci Instrum sive sampling of large-scale open quantum systems.

83:3881–3899.

18. Feynman RP (1992) There's plenty of room at the bot tom. J Microelectromech Svs 1(1):60–66

paths of inquiry. To cite just one exam-

notice that an MRFM cantilever and a microscopes having resonant ferromag-

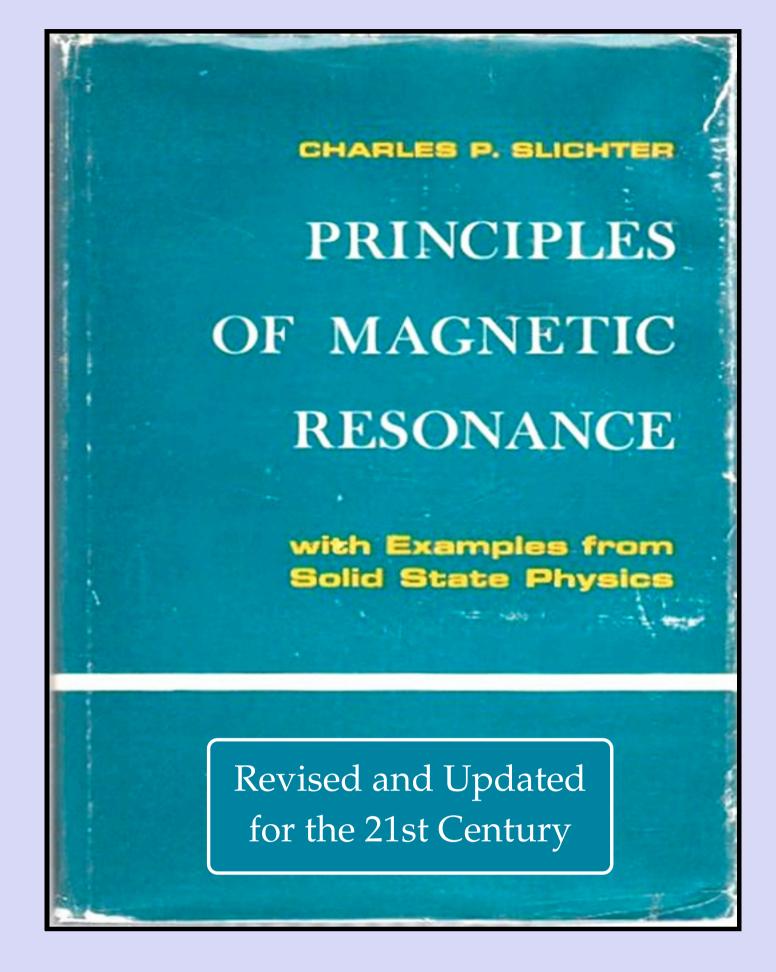
cesses in large magnetic gradients, with a view toward achieving by dynamical nuclear spin polarization an MRFM signal strength sufficient for imaging with  $(0.5 \text{ nm})^3$  voxel resolution, sufficient for the direct imaging of (for example) the changes in chromatin architecture that are associated to cell differentiation in regenerative healing processes.

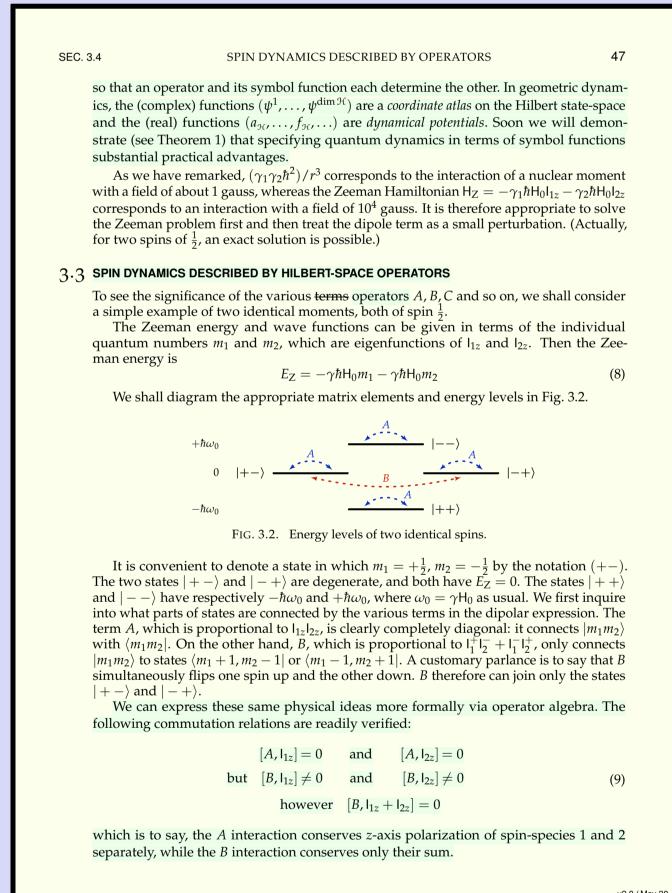
**Acknowledgements** This work is dedicated to the families of the Ceremony in Honor of Wounded Marines, 12 May 2006, Marine Corps Barracks, Washington, DC. This research is supported by the Army Research Office (ARO) under MURI program # W911NF-05-1-0403. Presented as poster #PA-15, 52nd ENC, April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

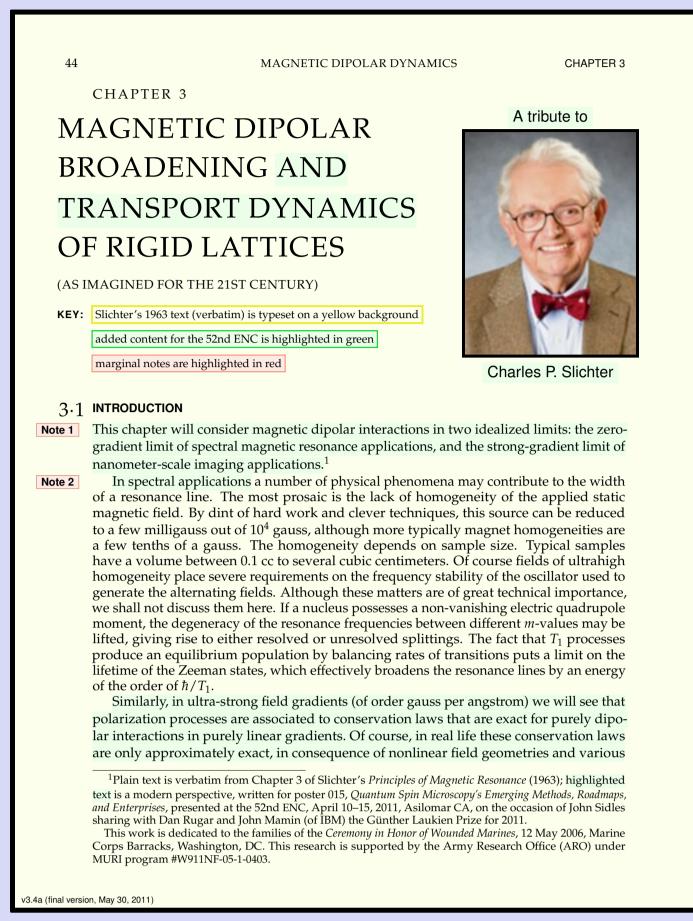
- [1] C. L. Degen, M. Poggio, H. J. Mamin, C. T. Rettner, and D. Rugar. Nanoscale magnetic resonance imaging. Proc. Nat. Acad. Sci. USA, 106(5):1313–1317, 2009. 2] J. Von Neumann. Letter to Norbert Wiener from John von Neumann. In V. Mandrekar and P. R. Masani, editors, Proceedings of the Norbert Wiener Centenary Congress, 1994, volume 52 of Proc. Symp. Appl. Math., pages 506-512. AMS, 1997.
- [3] J. A. Sidles. Spin microscopy's heritage, achievements, and prospects. Proc. Nat. Acad. Sci., 106(8):2477-8, 2009. [4] J. A. Sidles, J. L. Garbini, L. E. Harrell, A.O. Hero, J. P. Jacky, J. R. Malcomb, A. G. Norman, and A. M. Williamson. Practical recipes for the model order reduction, dynamical simulation, and

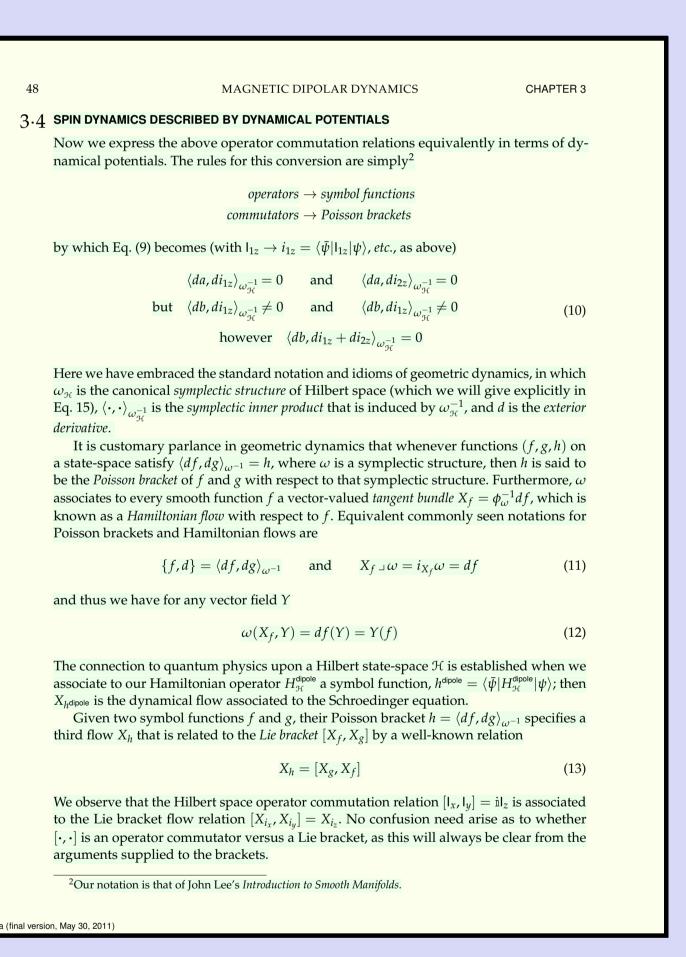
Prospects

- compressive sampling of large-scale open quantum systems. New Journal of Physics, 11(6):065002 (96pp), 2009.
- [5] J. A. Sidles, J. L. Garbini, J. P. Jacky, R. A. R. Picone, and S. A. Harsila. Elements of naturality in dynamical simulation frameworks for Hamiltonian, thermostatic, and Lindbladian flows on classical and quantum state-spaces. ArXiv e-prints, July 2010. arXiv:1007.1958.







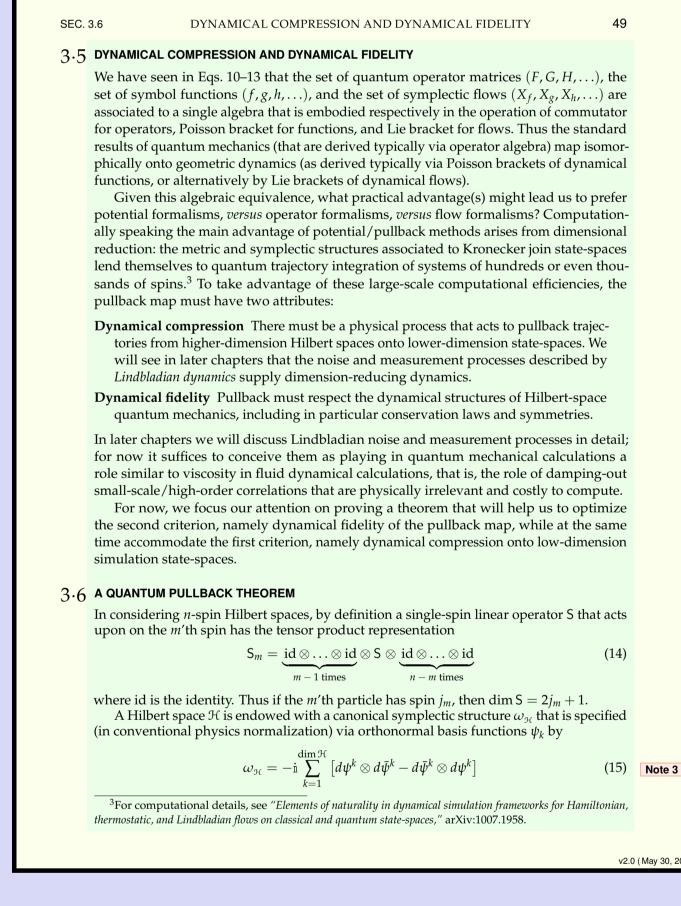


MAGNETIC DIPOLAR DYNAMICS

 $\gamma_{\mathsf{b}} 
ho_{\mathsf{b}} D_{\mathsf{ba}} = -\gamma_{\mathsf{a}} 
ho_{\mathsf{a}} D_{\mathsf{aa}}$ 

 $\gamma_{\mathsf{a}} \, \rho_{\mathsf{a}} D_{\mathsf{a}\mathsf{b}} = - \gamma_{\mathsf{b}} \, \rho_{\mathsf{b}} D_{\mathsf{b}\mathsf{b}}$ 

CHAPTER 3



non-dipole interactions (particularly for electrons)

detail without instrumental limitations.

and  $\mu_2$  as operators as usual:

of course, we exclude terms with i = k.

In this chapter, however, we shall ignore all these effects and concentrate on the

contribution of the magnetic dipole coupling between the various nuclei to the width

of the Zeeman transition. This approximation is often excellent, particularly when the

nuclei have spin  $\frac{1}{2}$  (thus a vanishing quadrupole moment) and a rather long spin-lattice

coupling is easily made. If typical neighboring nuclei are a distance r apart and have

By using  $r=2\,\text{Å}$  and  $\mu=10^{-23}\,\text{erg/gauss}$  (10<sup>-3</sup> of a Bohr magneton), we find H<sub>loc</sub>  $\simeq$ 

1 gauss. Since this field may either aid or oppose the static field H<sub>0</sub>, a spread in the

resonance conditions results, with significant absorption occurring over a range of  $H_0 \sim$ 

1 gauss. The resonance width on this argument is independent of  $H_0$ , but for typical

laboratory field of 10<sup>4</sup> gauss, we see there is indeed a sharp resonant line. Since the width

is substantially greater than the magnet inhomogeneity, it is possible to study the shape in

where r is the radius vector from  $\mu_1$  to  $\mu_2$  (the expression is unchanged if r is taken as the

vector from  $\mu_2$  to  $\mu_1$ .) If we regard  $\mu_1$  and  $\mu_2$  as coordinates on a classical state-space, then

For the quantum mechanical Hamiltonian operator we simply take Eq. (1), treating  $\mu_1$ 

where we have assumed that both the gyromagnetic rations and the spins may be different.

The general dipolar contribution to the Hamiltonian for N spins then becomes the operator

 $h_{_{\mathcal{H}}}^{\mathsf{dipole}} = \langle ar{\psi} | H^{\mathsf{dipole}} | \psi 
angle$ 

Mathematicians call  $h_H^{\text{dipole}}$  the symbol function of  $H^{\text{dipole}}$ . Here we are regarding Hibert space

as a state-space manifold  $\mathcal H$  that is equipped with a set of (complex) coordinate functions

 $(\psi_1, \dots, \psi_{\dim \mathcal{H}}, \bar{\psi}_1, \dots, \bar{\psi}_{\dim \mathcal{H}}) \colon \mathcal{H} \to \mathbb{C}$ ; thus symbol functions are *bilinear* in  $\bar{\psi}$  and  $\psi$ .

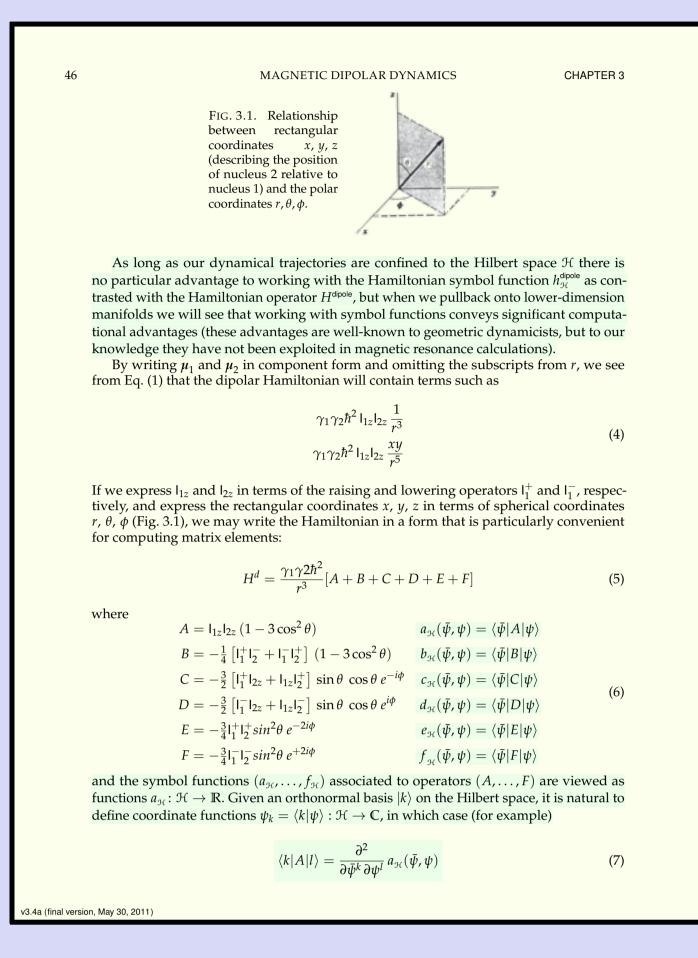
Associated to the Hamiltonian operator  $H^{\text{dipole}}$  is a potential function

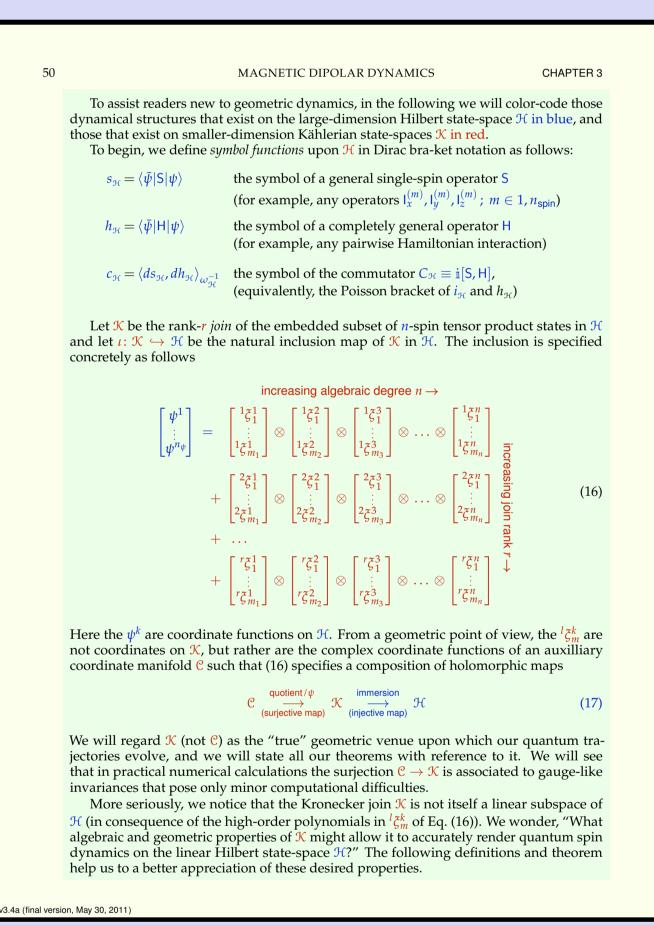
we recognize that Eq. 1 specifies *E* as the *Hamiltonian potential* on that state-space.

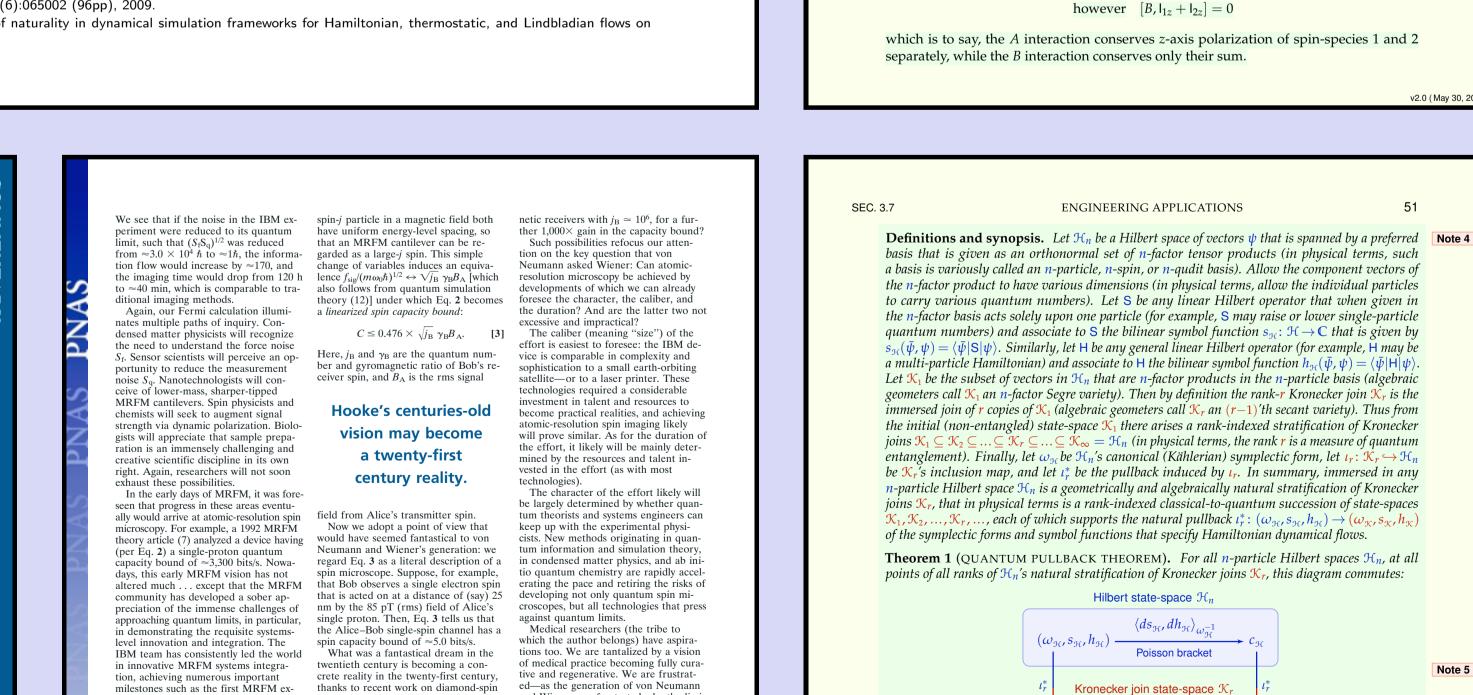
The classical interaction energy *E* between two magnetic moments  $\mu_1$  and  $\mu_2$  is

magnetic moment  $\mu$ , they produce a magnetic field  $H_{loc}$  of the order

Regardless of whether a gradient is present, a rough estimate of the effect of the dipolar







sire—as Feynman famously desired—to

'just look at the thing' (18). And we

magnetometry with diamond spins under ambient conditions. *Nature* 455:648–651.

plan—as every previous generation has

planned—for these aspirations to

