Spin microscopy's heritage, achievements, and prospects

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Achieving 3-dimensional, in-depth, atomic-resolution biological microscopy of undenatured specimens is one of the oldest dreams of science, and for good reason: it unites the thrilling prospect of opening vast new scientific frontiers with cutting-edge technical challenges from every domain of mathematics, science, and engineering.

In a recent issue of PNAS, a team from IBM Research led by Dan Rugar and John Mamin has taken us a giant step closer to this goal (1) by using magnetic resonance force microscopy (MRFM) to obtain 3-dimensional images of tobacco mosaic viruses having voxel resolution down to ≈4 nm. Our comments on the IBM experiment will be modeled on a 1946 letter from John von Neumann to Norbert Wiener (2), in which von Neumann discusses, at considerable length, both the practical problem of achieving atomic-resolution biological microscopy and the potential applications of this capability. Von Neumann's letter invites Wiener to consider whether 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?"

We adopt von Neumann's question as this commentary's focus, and we seek to describe paths by which mathematicians, scientists, and engineers—of almost every discipline—can contribute to, or benefit from, this centuries-old quest.

We begin by conceiving of spin microscopy in terms of communication: we regard sample spins as being modulated by Alice so as to create a signal force $f(t)$ that is observed by Bob (Fig. 1).

We ask the natural question, how fast can Alice transmit information to Bob? This rate, called the *channel capacity*, is rigorously bounded by Claude Shannon's 1949 Capacity Theorem as

$$C \leq 0.476 \times f_{\rm sig}/(m^2\omega_0^2 S_f S_q)^{1/4}. \qquad [1]$$

The meaning of these parameters and their values in the IBM experiments are as follows: Alice's root-mean-square force signal is $f_{\rm sig} \simeq 10$ aN, Bob's MRFM cantilever has mass $m \simeq 0.26$ ng, frequency $\omega_0/(2\pi) \simeq 2.9$ kHz, force noise $S_f^{1/2} \simeq 10$ aN/$\sqrt{\rm Hz}$ (one-sided), and measurement noise $S_q^{1/2} \simeq 1.0$ pm/$\sqrt{\rm Hz}$. The coefficient 0.476 is the extremum of *Shannon's waterfilling integral* (equation 32 in ref. 4) for $S_{\rm f}$ and $S_{\rm q}$ varied with $S_{\rm f}S_{\rm q}$ held fixed.

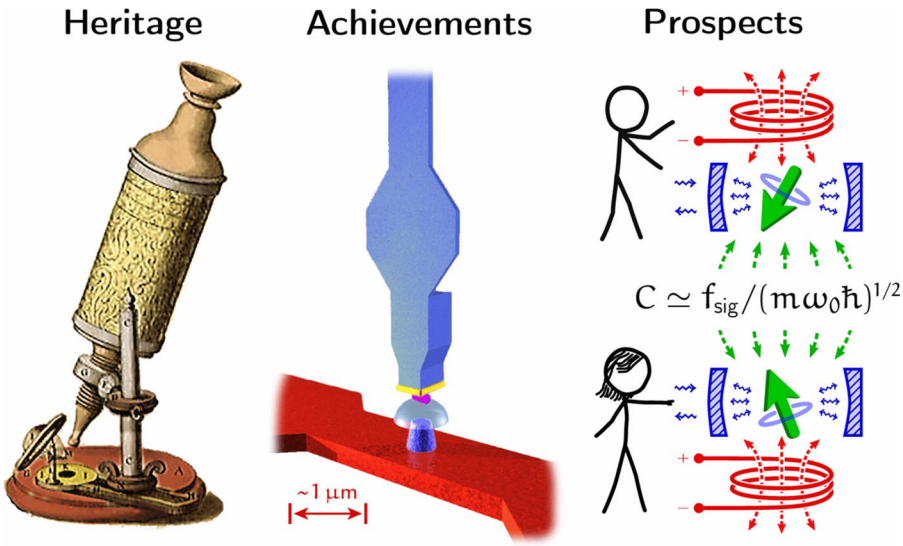

Fig. 1. Spin microscopy continues a heritage that began with Robert Hooke's 1667 vision that (3) "by the help of microscopes, there is nothing so small, as to escape our inquiry" (*Left*). The imaging achievements of the IBM Research Division (*Center*) extend and strengthen this heritage. These achievements lead us to 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 information science, and many other disciplines—advances that in aggregate are transforming present conceptions of microscopy—Hooke's centuries-old vision may become a twenty-first century reality (Alice and Bob figures by permission of www.xkcd.com).

Inserting these IBM device parameters into Eq. **1**, we compute a capacity bound of $C \lesssim 40$ bits/s. This figure-of-merit, and elaborations of it, will be the main focus of this commentary. Von Neumann and Wiener would recognize this approach as a *Fermi calculation*, and perhaps would be pleased that the methods of their colleague Enrico Fermi are now regarded as essential to design and systems engineering (5).

Multiple paths of inquiry depart from this Fermi calculation starting point. Communication theorists will recognize that a stronger capacity bound is obtained by specifying $S_{\rm f}$ and $S_{\rm q}$ individually, rather than constraining only their product $S_{\rm f}$ $S_{\rm q}$ as in Eq. **1**. The resulting expression is more complicated than Eq. **1** (and is not given here) but the bound obtained is not much stronger: $C \lesssim 8.5$ bits/s. This means that the IBM team has balanced force and measurement noise nearly optimally. Good.

Imaging researchers will appreciate that 8.5 bits/s is painfully slow, equivalent to transmitting a 90-kB image file in 24 h. Together with inevitable real-world inefficiencies, this explains the lengthy 120-h acquisition time of the IBM images (1). Slow imaging is a generic challenge in magnetic resonance, and an array of remediating techniques stand ready to be applied, including signal multiplexing, incorporation of ab initio information into modulation and deconvolution algorithms, and (very recently) sparse sampling. Researchers will not soon exhaust these possibilities.

It is good to acquire data faster, so let us now consider paths for boosting the raw channel capacity of Eq. **1**.

Quantum information researchers will recognize that the noise product $S_{\rm f}S_{\rm q}$ is subject to a fundamental (and rigorous) inequality $S_{\rm f}S_{\rm q} \geq \hbar^2$ (one-sided) (equation 6.7 in ref. 6), which is called the *standard quantum limit* (SQL). Eq. **1** then implies the *test-mass capacity bound*

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

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We see that if the noise in the IBM experiment were reduced to its quantum limit, such that $(S_f S_q)^{1/2}$ was reduced from $\approx 3.0 \times 10^4\ \hbar$ to $\approx 1\hbar$, the information flow would increase by ≈170, and the imaging time would drop from 120 h to ≈40 min, which is comparable to traditional imaging methods.

Again, our Fermi calculation illuminates multiple paths of inquiry. Condensed matter physicists will recognize the need to understand the force noise S_f. Sensor scientists will perceive an opportunity to reduce the measurement noise S_q. Nanotechnologists will conceive of lower-mass, sharper-tipped MRFM cantilevers. Spin physicists and chemists will seek to augment signal strength via dynamic polarization. Biologists will appreciate that sample preparation is an immensely challenging and creative scientific discipline in its own right. Again, researchers will not soon exhaust these possibilities.

In the early days of MRFM, it was foreseen that progress in these areas eventually would arrive at atomic-resolution spin microscopy. For example, a 1992 MRFM theory article (7) analyzed a device having (per Eq. **2**) a single-proton quantum capacity bound of ≈3,300 bits/s. Nowadays, this early MRFM vision has not altered much . . . except that the MRFM community has developed a sober appreciation of the immense challenges of approaching quantum limits, in particular, in demonstrating the requisite systems-level innovation and integration. The IBM team has consistently led the world in innovative MRFM systems integration, achieving numerous important milestones such as the first MRFM experiment (8), the first detection of statistical polarization by MRFM (9), the first detection of gradient suppression of spin diffusion (10), the first MRFM detection and imaging of a single (electron) spin (11), and now the first high-resolution MRFM biological images (1).

Let us consider one final Fermi calculation, with a view toward illuminating some of the paths that lie ahead. We notice that an MRFM cantilever and a spin-j particle in a magnetic field both have uniform energy-level spacing, so that an MRFM cantilever can be regarded as a large-j spin. This simple change of variables induces an equivalence $f_{sig}/(m\omega_0\hbar)^{1/2} \leftrightarrow \sqrt{j_B}\ \gamma_B B_A$ [which also follows from quantum simulation theory (12)] under which Eq. **2** becomes a *linearized spin capacity bound*:

$$C \leq 0.476 \times \sqrt{j_B}\ \gamma_B B_A. \qquad [3]$$

Here, j_B and γ_B are the quantum number and gyromagnetic ratio of Bob's receiver spin, and B_A is the rms signal field from Alice's transmitter spin.

Hooke's centuries-old vision may become a twenty-first century reality.

Now we adopt a point of view that would have seemed fantastical to von Neumann and Wiener's generation: we regard Eq. **3** as a literal description of a spin microscope. Suppose, for example, that Bob observes a single electron spin that is acted on at a distance of (say) 25 nm by the 85 pT (rms) field of Alice's single proton. Then, Eq. **3** tells us that the Alice–Bob single-spin channel has a spin capacity bound of ≈5.0 bits/s.

What was a fantastical dream in the twentieth century is becoming a concrete reality in the twenty-first century, thanks to recent work on diamond-spin imaging (13–16) that has greatly expanded our conception of the challenges and opportunities of quantum spin microscopy (17).

Now for the third time our Fermi calculation (Eq. **3**) illuminates multiple paths of inquiry. To cite just one example: the obvious parameter to improve in Eq. **3** is the quantum number j_B. Ought we to begin conceiving of spin microscopes having resonant ferromagnetic receivers with $j_B \simeq 10^6$, for a further 1,000× gain in the capacity bound?

Such possibilities refocus our attention on the key question that von Neumann asked Wiener: Can atomic-resolution microscopy 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?

The caliber (meaning "size") of the effort is easiest to foresee: the IBM device is comparable in complexity and sophistication to a small earth-orbiting satellite—or to a laser printer. These technologies required a considerable investment in talent and resources to become practical realities, and achieving atomic-resolution spin imaging likely will prove similar. As for the duration of the effort, it likely will be mainly determined by the resources and talent invested in the effort (as with most technologies).

The character of the effort likely will be largely determined by whether quantum theorists and systems engineers can keep up with the experimental physicists. New methods originating in quantum information and simulation theory, in condensed matter physics, and ab initio quantum chemistry are rapidly accelerating the pace and retiring the risks of developing not only quantum spin microscopes, but all technologies that press against quantum limits.

Medical researchers (the tribe to which the author belongs) have aspirations too. We are tantalized by a vision of medical practice becoming fully curative and regenerative. We are frustrated—as the generation of von Neumann and Wiener was frustrated—by the limitations of our present tools. We desire—as Feynman famously desired—to "just look at the thing" (18). And we plan—as every previous generation has planned—for these aspirations to become realities.

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