

# REALISTIC SIMULATIONS OF SINGLE-SPIN MEASUREMENT VIA MAGNETIC RESONANCE FORCE MICROSCOPY\*

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The problem of measuring single electron or nuclear spins is of great interest for a variety of purposes, from imaging the structure of molecules to quantum information processing. One of the most promising techniques is magnetic resonance force microscopy (MRFM), in which the force between a spin and a small permanent magnet resonantly drives the oscillations of a microcantilever. Numerous issues arise in understanding this system: thermal noise in the cantilever, shot-noise and back-action from monitoring the cantilever's motion, spin relaxation, and interaction with higher cantilever modes. Detailed models of these effects allow one to assess their relative importance and the necessary improvements for sensitivity at the single-spin level.

## 1. Single spin measurement

Single-spin measurement is an extremely important and difficult challenge for modern quantum technology. It is necessary for the success of several spin-based proposals for quantum information processing<sup>1,2,3,4,5</sup>. Single spin detection can be done either *indirectly*, by turning the spin measurement into the movement of a charge (using, e.g., a single-electron transistor); or *directly* by detecting the force produced by the spin's magnetic field. For direct measurement, the most promising approach is magnetic resonance force microscopy (MRFM)<sup>6,7,8</sup>.

MRFM has recently reached the sensitivity to detect (but not measure) a single electron spin—a feat which AIP Physics News recently called the top story of 2004<sup>9</sup>. We should note, however, that even “direct” detection is really indirect.

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The forces exerted by a single spin are far too weak to be detected by macroscopic devices without a lot of clever tricks!

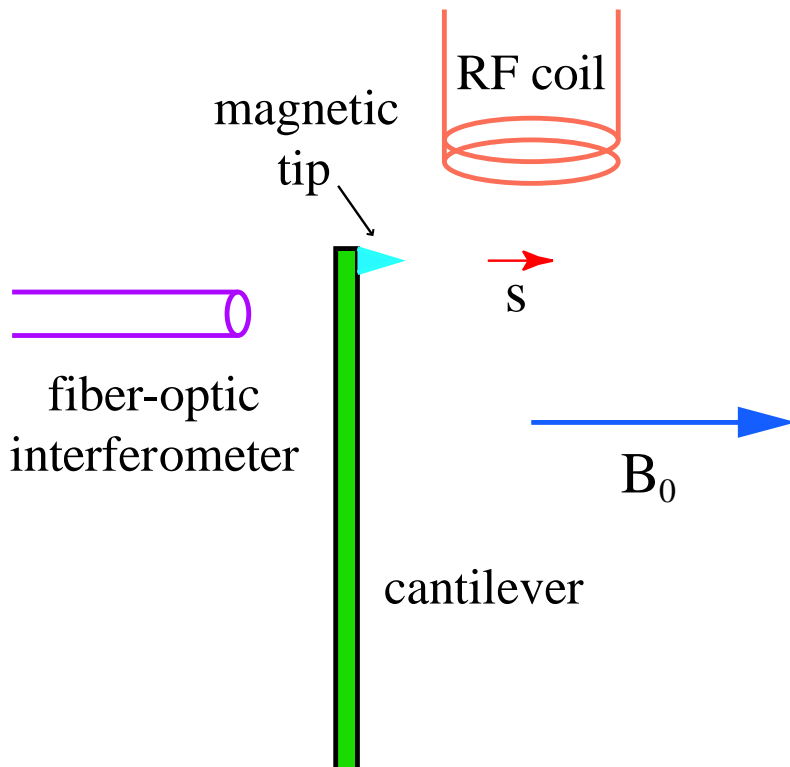


Figure 1. A schematic diagram of the setup for an MRFM spin measurement.

## 2. Cyclic adiabatic inversion

For this paper, we will mostly discuss a version of this protocol called *Cyclic Adiabatic Inversion*<sup>8,10,11,12</sup> (CAI). The spin of the electron precesses in a local magnetic field with three components: an imposed external field; the field from a permanent magnet on the tip of a nearby high- $Q$  microcantilever; and the field from incident microwaves.

The microwave field is given a frequency modulation in resonance with the cantilever. The precessing spin moves adiabatically with the field. The electron spin has a dipole-dipole interaction with the permanent magnet, thereby exerting a

weak force, which varies periodically in resonance with the cantilever. Over many oscillations, the cantilever is driven by this force until it produces an amplitude which is detectable by an optical interferometer.

The initial orientation of the spin will determine the sign of this driving force. Thus, the output signal is the phase of the resulting cantilever oscillations. These in turn produce an oscillating photocurrent in the optical interferometer. It is this photocurrent which is actually measured. This chain of successive amplifications reminds one of the remarkable inventions of Rube Goldberg. An oscillating spin produces over time an oscillating cantilever, which in turn produces an optical signal, which is finally read out as a photocurrent.

The Hamiltonian which describes the interaction of the spin and the cantilever is

$$\hat{H}_{SZ}(t) = \hat{H}_Z - 2\eta\hat{Z}\hat{S}_z + f(t)\hat{S}_z - \varepsilon\hat{S}_x, \quad (1)$$

$$\hat{H}_Z = \frac{1}{2m}\hat{p}^2 + \frac{m\omega_m^2}{2}\hat{Z}^2. \quad (2)$$

Because  $f(t)$  and  $\varepsilon$  are both large compared to the cantilever frequency  $\omega_m$ , we can switch to a rotating picture and make a rotating wave approximation. In this approximation the Hamiltonian becomes

$$H'_{SZ}(t) = \hat{H}_Z - 2\eta g(t)\hat{Z}\hat{S}'_z, \quad (3)$$

where  $\hat{S}'_z$  is the transformed spin operator and  $g(t) = f(t)/\sqrt{f^2(t) + \varepsilon^2}$  is a new periodic function which is still resonant with the cantilever.

We seen from this Hamiltonian that if the spin is initially in the  $\pm 1/2$  eigenstate of  $\hat{S}'_z$ , it remains in that state at all successive times; and this state determines the sign of the driving force acting on the oscillator.

As Fig. 2 shows, the rotating-wave approximation is quite accurate. The measurement is made by looking at the phase of the cantilever oscillation. We see in Fig. 3 that the components at different phases change quite markedly with time, depending on the orientation of the measured spin.

### 3. Modeling MRFM

To model the complete MRFM measurement process we need more than just the spin-cantilever Hamiltonian. We need to include three degrees of freedom: the cantilever, the spin, and the optical cavity mode. We need to include *thermal noise and damping* in the cantilever, *cavity loss* in the cavity, and the *effects of monitoring* (i.e., measurement back-action).

Because optical frequencies are much higher than spin precession or cantilever oscillation, and the cavity is highly lossy, the cavity mode degree of freedom can

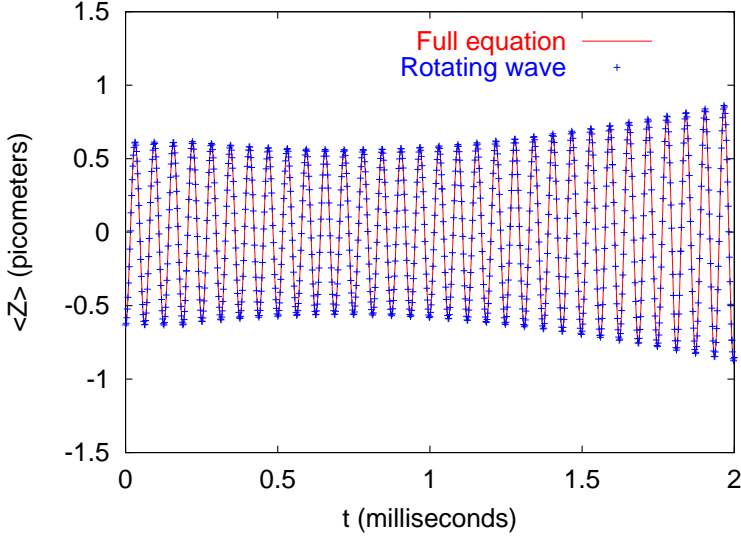


Figure 2. A comparison between the full equations and the rotating-wave approximation for an MRFM system.

be adiabatically eliminated. The result is a *stochastic master equation* for the spin and cantilever degrees of freedom<sup>13,14</sup>.

The stochastic master equation is

$$d\rho = -\frac{i}{\hbar}[\hat{H}, \rho]dt + \sum_j (2\hat{L}_j \rho \hat{L}_j^\dagger - \{\hat{L}_j^\dagger \hat{L}_j, \rho\})dt + \sqrt{2e_d} ((\hat{L}_2 - \langle \hat{L}_2 \rangle)\rho + \rho(\hat{L}_2 - \langle \hat{L}_2 \rangle)) dW_t . \quad (4)$$

$$M[dW_t] = 0, \quad M[(dW_t)^2] = dt . \quad (5)$$

The Lindblad operators are

$$\begin{aligned} \hat{L}_1 &= \sqrt{\gamma_m/2} ((1/\ell)\hat{Z} + i(\ell/\hbar)\hat{p}) , \\ \hat{L}_2 &= \sqrt{8\kappa^2 E^2/\gamma_c^3} \hat{Z} , \end{aligned} \quad (6)$$

and the effective Hamiltonian is

$$\hat{H}(t) = \hat{H}'_{SZ}(t) + \frac{4\kappa E^2}{\gamma_c^2} \hat{Z} + (\gamma_m/2)(\hat{Z}\hat{p} + \hat{p}\hat{Z}) . \quad (7)$$

The  $\hat{L}_2$  terms are the result of monitoring, and produce a stochastic localization<sup>15</sup> of the cantilever position  $Z$ .

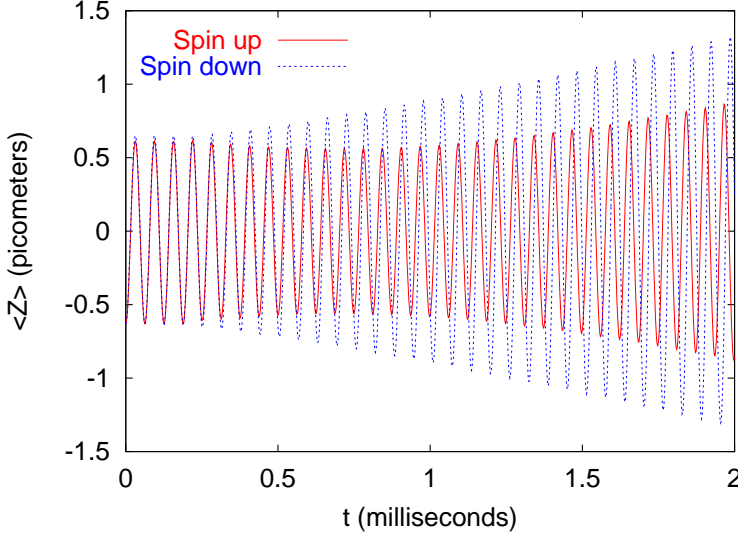


Figure 3. Cantilever position versus time for spin up and spin down.

Because the cantilever position is driven by the sign of the spin, however, this localization in position also produces a localization in the spin  $\hat{S}'_z$ .

This localization is very fast! In fact, as we can see from Fig. 4, it takes place long before we can actually detect the signal which indicates the spin orientation (since that takes many cantilever oscillations).

#### 4. Stochastic Schrödinger Equation

Solving the stochastic master equation is possible numerically, but in practice is very difficult. It turns out to be far more efficient to *unravel* this master equation into a *stochastic Schrödinger equation* (SSE).

$$\begin{aligned}
 d|\psi\rangle = & -\frac{i}{\hbar}\hat{H}(t)|\psi_{SZ}\rangle dt + \sum_{j=1}^2 \left( 2\langle\hat{L}_j^\dagger\rangle\hat{L}_j - \hat{L}_j^\dagger\hat{L}_j - |\langle\hat{L}_j\rangle|^2 \right) |\psi_{SZ}\rangle dt \\
 & + \sqrt{2}(\hat{L}_1 - \langle\hat{L}_1\rangle) |\psi_{SZ}\rangle dW_{1t} + \sqrt{2e_d}(\hat{L}_2 - \langle\hat{L}_2\rangle) |\psi_{SZ}\rangle dW_{2t} \\
 & + \sqrt{2(1-e_d)}(\hat{L}_2 - \langle\hat{L}_2\rangle) |\psi_{SZ}\rangle dW_{3t}. \quad (8)
 \end{aligned}$$

By averaging over  $W_1$  and  $W_3$  we can reproduce the solution to the stochastic master equation. The advantage of an SSE is that we can take advantage of *localizing effects* which tend to make the solutions remain small wavepackets at all times.

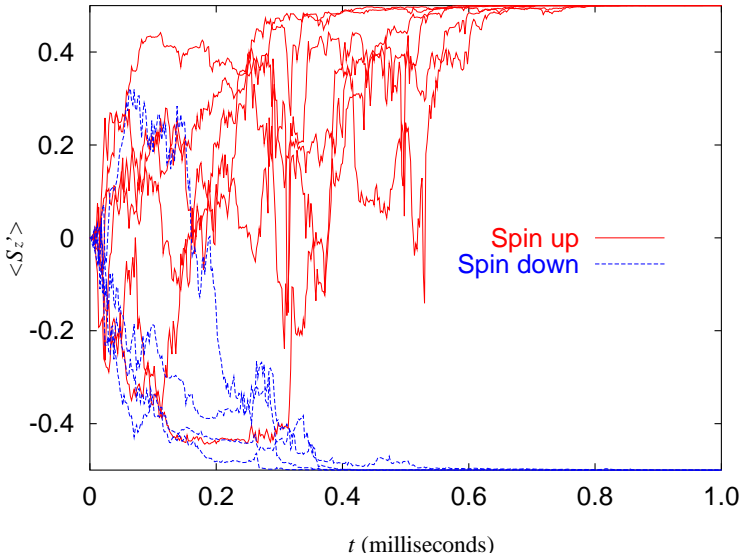


Figure 4. The expectation value of spin  $\langle \hat{S}_z \rangle$  as a function of time for ten different trajectories, where the initial spin is in the superposition  $(|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$ . Note that the spins randomly settle on either the state up or down in a short time.

In fact, we might use this tendency to further simplify our description. Suppose that we assume that the state of the cantilever plus spin is

$$|\psi\rangle = \sqrt{r}|\phi_d\rangle|\downarrow\rangle + \sqrt{1-r}|\phi_u\rangle|\uparrow\rangle, \quad (9)$$

and  $|\phi_d\rangle$  and  $|\phi_u\rangle$  remain small Gaussian wavepackets at all times. What kind of description does that give us? We can find a set of coupled differential equations for the wave packet positions and momenta and the spin probability  $r$ .

These equations look like this:

$$\begin{aligned} dZ_d &= (p_d/m)dt + \text{extra terms}, \\ dp_d &= (-m\omega_m^2 Z_d - \eta g(t) - 2\gamma_m p_d)dt + \text{extra terms}, \\ dZ_u &= (p_u/m)dt + \text{extra terms}, \\ dp_u &= (-m\omega_m^2 Z_u + \eta g(t) - 2\gamma_m p_u)dt + \text{extra terms}, \\ dr &= 2A(Z_u - Z_d)r(1-r)dW_t. \end{aligned} \quad (10)$$

The important point is that the leading terms of these equations are just like the classical equations for damped driven oscillators, and  $r \rightarrow 0, 1$  at long times. Because these equations mirror the classical equations, it turns out that estimates of

this system's behavior based on classical intuition are actually surprisingly accurate. The two curves are plotted in Fig. 5 for the same realization of the noise, and are extremely close.

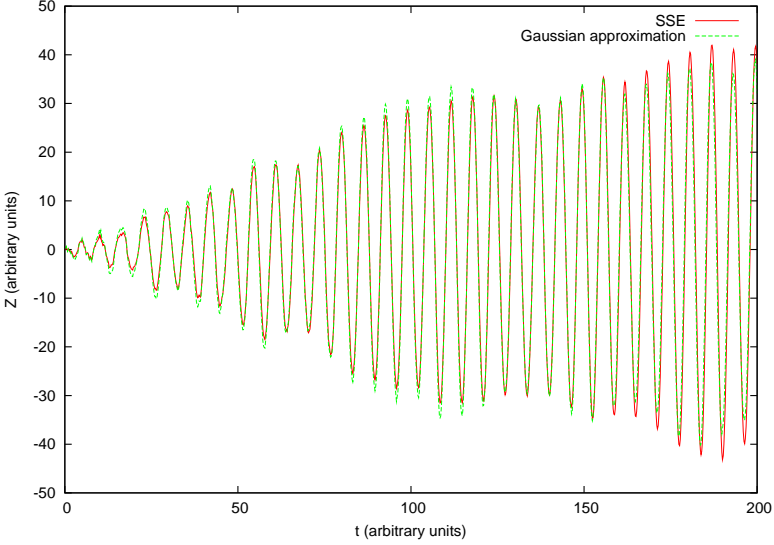


Figure 5. A comparison between the fully quantum equations and the Gaussian approximation for an MRFM system.

## 5. Spin relaxation and quantum jumps

We have considered several sources of error on the cantilever. To accurately model the real physical system, however, we must also include noise which affects the *spin*. The simplest type we might consider is *spin relaxation*, in which we add to our stochastic master equation terms corresponding to a Lindblad operator of the form

$$\hat{L}_S = \sqrt{1/t_1} \hat{S}'_x. \quad (11)$$

This represents noise in the local environment of the spin which tends to flip its orientation. To be a reasonable measurement technique, our MRFM setup must be able to measure the spin in a time short compared to  $t_1$ .

At present we are not very close to that limit. In the recent single-spin detection experiment, the signal was obtained by averaging data over 13 *hours*. By contrast, the spin relaxation time was on the order of hundreds of milliseconds.

However, improving sensitivity by one or two orders of magnitude would make a dramatic difference in the time needed to produce a signal. At that point, true single-spin measurements will be possible.

We can unravel the effects due to spin relaxation as well, to recover a new SSE. In this case, it is convenient to use a different kind of unraveling, into *quantum jumps*. The new SSE contains a term

$$d|\psi\rangle = \dots + (\hat{S}'_x - 1)|\psi\rangle dN, \quad (12)$$

where  $dN^2 = dN$  and  $M[dN] = dt/t_1$ . This term is usually zero; but randomly, with rate  $1/t_1$ , quantum jumps occur. In a jump,  $dN = 1$  and the spin orientation is flipped. This SSE is a hybrid form of stochastic equation, containing both diffusive and jump terms.

In the Gaussian approximation, this effect is easily incorporated by having a rate for jumps which switch the “up” and “down” wavepackets, causing  $Z_d, p_d \leftrightarrow Z_u, p_u$  and  $r \rightarrow 1 - r$ .

## 6. What's left?

At present we include many important effects in our model: thermal noise, measurement back-action, shot-noise and spin-relaxation. What remains to be done?

- (1) Actual spin-relaxation need not take the simple form described above; simple noise in the lab frame can become time dependent in the rotating frame.
- (2) Recent experiments use a different protocol than CAI, called OSCAR. Our model must be adapted to this different technique.
- (3) Interaction between the spin and higher modes of the cantilever is a significant source of noise. This should be included.
- (4) In the longer term, we'd like to treat systems with multiple nearby spins.

In general, the goal would be to develop models of sufficient accuracy to help experimenters in assessing the relative merits of different protocols, and perhaps to find the most useful areas for improvement. There is a large gap, at present, between what is theoretically possible and what is experimentally feasible; an important need is to develop the theoretical and numerical tools to help fill that gap.

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