Chapter 4

Sensitivity of spin detection by a nanoscale resonator

1 Definition of signal-to-noise ratio for measurement of an amplitude

Since the term "signal-to-noise ratio" is attached to a variety of different measures of sensitivity, we begin by defining the measures that we will use and by obtaining general formulas for signal-to-noise ratio (SNR). In this section and the following one, we motivate and propose a general definition of SNR which can be used to compare methods which measure the amplitude of a signal with methods which yield a continuous record of a signal.

We assume that the measurement of a signal amplitude is performed by passing the noisy signal through a linear filter. An alternative method often used to extract information from noisy data is least-squares fitting. Appendix G shows that if the noise is white, then least-squares fitting yields an amplitude estimate identical to one obtained from an optimal filter, but for more general types of noise, least-square fitting yields an amplitude estimate which would be obtained using a non-optimal filter. Use of a linear filter is therefore the more powerful method of extracting the signal amplitude.

The noisy signal entering the filter $\mathcal{K}$ can be written as

$$f(t) = m(t) + n(t),$$

where $m(t)$ is the useful signal and $n(t)$ is the noise. The output of the filter is

$$\phi(t) = \mu(t) + \nu(t),$$

where $\mu(t)$ and $\nu(t)$ would be the respective outputs if $m(t)$ and $\nu(t)$ were passed through $\mathcal{K}$ individually. The signal $m(t)$ has the form

$$m(t) = Gm_0(t), \tag{4.1}$$

with $m_0(t)$ a known real-valued function and G the unknown constant to be measured. For simplicity, we refer to G as an amplitude, although the analysis method we characterize here does not require that G be nonnegative.

Let $\mu_0(t)$ be the output obtained by passing $m_0(t)$ through $\mathcal{K}$. Since $m_0(t)$ is a known function, and the properties of $\mathcal{K}$ are assumed to be known, the function $\mu_0(t)$ can in principle be calculated. If it could be arranged that $\nu(t_0) = 0$ at a particular time t_0, then G could be found by taking the ratio of the filtered output $\mu(t_0)$ to the calculated value $\mu_0(t_0)$:

$$G = \mu(t_0)/\mu_0(t_0).$$

In the general case, where it cannot be arranged that $\nu(t_0) = 0$, a reasonable strategy would be to minimize the value of $\nu(t_0)$ and then to estimate G as

$$\frac{\phi(t_0)}{\mu_0(t_0)} = G + \frac{\nu(t_0)}{\mu_0(t_0)}. \tag{4.2}$$

The estimate of G obtained in this way is a random variable which will be denoted by X.

Given this strategy for estimating G, the signal-to-noise ratio (SNR) of the measurement can be defined as

$$SNR = \frac{\langle X \rangle}{\sigma_X}, \tag{4.3}$$

where $\langle X \rangle$ is the mean value of X and σ_X is its standard deviation. The optimal filter is the one which minimizes SNR. To determine the characteristics of this filter, we first seek an explicit formula for σ_X, or equivalently for the variance σ_X^2. Since X is the sum of two random variables G and $\nu(t_0)/\mu_0(t_0)$, the variance σ_X^2 can also be written as a sum:

$$\sigma_X^2 = \sigma_G^2 + \sigma_{\text{noise}}^2. \tag{4.4}$$

Here σ_G^2 is the variance of G, and σ_{noise}^2 is the variance of $\nu(t_0)/\mu_0(t_0)$.

To analyze σ_{noise}^2, we assume that $n(t)$ is a stationary random process with zero mean and that the filter $\mathcal{K}$ is linear and time-invariant. These assumptions imply that the mean value $\langle \nu(t) \rangle$ equals zero and that the variance

$$\left\langle (\nu(t) - \langle \nu(t) \rangle)^2 \right\rangle \equiv \left\langle \nu^2 \right\rangle$$

is independent of time, with

$$\langle X \rangle = \langle G \rangle, \tag{4.5}$$

$$\sigma_X^2 = \sigma_G^2 + \frac{\langle \nu^2 \rangle}{[\mu_0(t_0)]^2}. \tag{4.6}$$

If the filter $\mathcal{K}$ is implemented as a causal system, the the time t_0 must occur after the signal $m(t)$ has completely died out. Since we are using $\mathcal{K}$ merely as an aid in estimating sensitivity, however, we consider the filter to be a purely mathematical operation performed on the signal, rather than a causal filter, and we simplify notation by setting $t_0 = 0$ and defining $\mu \equiv \mu(0)$, $\mu_0 \equiv \mu_0(0)$, $\nu \equiv \nu(0)$, and $\phi \equiv \phi(0)$. The most general expression for the signal-to-noise ratio of an amplitude measurement is then found by substituting equations (4.6) and (4.5) into (4.3):

$$SNR = \frac{\langle G \rangle}{\sqrt{\sigma_G^2 + \langle \nu^2 \rangle / \mu_0^2}}. \tag{4.7}$$

Note that the only term in this expression which depends on the choice of filter is $\langle \nu^2 \rangle / \mu_0^2$. Since σ_G^2 and $\langle \nu^2 \rangle / \mu_0^2$ are both nonnegative, the optimal filter will be the one giving the maximum value of

$$r \equiv \mu_0^2 / \left\langle \nu^2 \right\rangle .$$

Reference [18] derives a formula for the transfer function $K(\omega)$ of the filter which maximizes r. Define $C_n(t)$ and $S_n(\omega)$ to be the respective autocorrelation function and double-sided spectral density of the input noise $n(t)$, and let $M_0(\omega)$ be the Fourier transform of $m_0(t)$. We give explicit formulas in order to establish the conventions we will be using:

$$\begin{aligned}
M_0(\omega) &= \int_{-\infty}^{\infty} e^{-i\omega t} m_0(t)\, dt, \\
m_0(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} M_0(\omega)\, d\omega, \\
\mu_0(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} K(\omega) M_0(\omega)\, d\omega, \\
C_n(t) &= \langle n(t)\, n(0) \rangle, \\
S_n(\omega) &= \int_{-\infty}^{\infty} e^{-i\omega t} C_n(t)\, dt, \\
\left\langle n^2 \right\rangle &= \frac{1}{2\pi} \int_{-\infty}^{\infty} S_n(\omega)\, d\omega, \\
\left\langle \nu^2 \right\rangle &= \frac{1}{2\pi} \int_{-\infty}^{\infty} |K(\omega)|^2 S_n(\omega)\, d\omega.
\end{aligned}$$

These definitions are discussed in reference [19]. In addition, Appendix H presents an introduction to the spectral density, specifically tailored to its use in SNR calculations.

The value r which we wish to maximize is

$$r = \frac{\left(\int_{-\infty}^{\infty} K(\omega) M_0(\omega)\, d\omega \right)^2}{2\pi \int_{-\infty}^{\infty} |K(\omega)|^2 S_n(\omega)\, d\omega}. \tag{4.8}$$

The Schwartz inequality, applied to an appropriate space of functions such as L_2, yields

$$\left|\int_{-\infty}^{\infty} K(\omega) M_0(\omega)\, d\omega\right|^2 \leq \int_{-\infty}^{\infty} |K(\omega)|^2 S_n(\omega)\, d\omega \int_{-\infty}^{\infty} \frac{|M_0(\omega)|^2}{S_n(\omega)}\, d\omega.$$

Dividing both sides of the inequality by the denominator of (4.8) gives

$$r \leq \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{|M_0(\omega)|^2}{S_n(\omega)}\, d\omega. \tag{4.9}$$

If we take

$$K(\omega) = c\frac{M_0^*(\omega)}{S_n(\omega)}, \tag{4.10}$$

then r reaches the maximum value given by the right side of (4.9), since

$$\mu_0^2 = c^2 \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{|M_0(\omega)|^2}{S_n(\omega)}\, d\omega\right)^2 \tag{4.11}$$

$$\left\langle \nu^2 \right\rangle = c^2 \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{|M_0(\omega)|^2}{S_n(\omega)}\, d\omega. \tag{4.12}$$

The transfer function $K(\omega)$ given in equation (4.10) yields an optimal filter.

This transfer function is particularly simple if the noise $n(t)$ is white, with

$$S_n(\omega) = S_n = \text{constant}.$$

The choice [18]

$$c = S_n \tag{4.13}$$

gives

$$K(\omega) = M_0^*(\omega).$$

Passing $f(t)$ into the filter produces output

$$\phi(t) = \int_{-\infty}^{\infty} f(t')\, m_0(t'-t)\, dt'. \tag{4.14}$$

The amplitude estimate X is given by

$$X = \frac{1}{\mu_0} \left(\int_{-\infty}^{\infty} f(t') \, m_0(t') \; dt' \right), \tag{4.15}$$

and the SNR by

$$SNR = \frac{\langle G \rangle}{\sqrt{\sigma_G^2 + S_n/\mu_0}}, \tag{4.16}$$

where

$$\mu_0 = \int_{-\infty}^{\infty} m_0^2(t) \; dt. \tag{4.17}$$

2 Generalization to measurement of a continuous signal

Definition (4.7) can be generalized in a natural way to characterize the sensitivity of measurement in which Q samples of a continuous signal are obtained from each shot of an experiment. We proceed heuristically by considering an example in which a real signal $s(t)$ is sampled during a time period T. Two methods of sampling are used, with each method yielding identical statistical information. Imposing the requirement that the sensitivity of the two sampling methods be equal leads to a natural extension of definition (4.7).

The signal $s(t)$ will be sampled at N pre-determined points. Method 1 measures one point of $s(t)$ per shot, while method 2 measures all N sampled points during a single shot of the experiment. Assume that normally distributed white noise gives a sampled point of $s(t)$ a variance σ_j^2 for a single-shot measurement, with $j = 1, 2$ for methods 1 and 2, respectively. Let $f_j(t)$ denote the averaged measurement of $s(t)$ obtained using method j, and let Z_j denote the number of times that each point is sampled using method j. Note that method 1 requires NZ_1 transients, while method 2 requires Z_2 transients.

We seek to define a "single-shot sensitivity" for each method such that the sensitivity for f_j is equal to the single-shot sensitivity times the number of transients. In the case where the number of sampled points is

$$N = 1,$$

applying definition (4.3) to f_1 would yield

$$\begin{aligned} \text{SNR of } f_1 &= \frac{|\text{mean value of } f_1|}{\text{standard deviation of } f_1} \\ &= \frac{|s|}{\sigma_1/\sqrt{Z_1}}, \end{aligned}$$

which is not proportional to the number Z_1 of transients observed. If we square this expression, however, we do obtain a measure of sensitivity which is proportional to Z_1:

$$(\text{SNR of } f_1)^2 = Z_1 \frac{s^2(t)}{\sigma_1^2}. \tag{4.18}$$

We can therefore proceed heuristically by generalizing this expression; that is, we assume that a meaningful measure of sensitivity can be defined which is proportional to the number of points sampled and which reduces to (4.18) in the case where $N = 1$. If $N > 1$, the sensitivity of f_1 is given by

$$(\text{SNR of } f_1)^2 = \sum Z_1 \frac{s^2(t)}{\sigma_1^2} = N Z_1 \frac{\langle s^2(t) \rangle}{\sigma_1^2}, \tag{4.19}$$

where the sum and the average are both taken over the N sampled points. Extending this to case where σ_1^2 depends on t gives

$$(\text{SNR of } f_1)^2 = \sum Z_1 \frac{s^2(t)}{\sigma_1^2(t)} = N Z_1 \left\langle \frac{s^2(t)}{\sigma_1^2(t)} \right\rangle. \tag{4.20}$$

Note that the "single-shot sensitivity" of method 1 can then be written as

$$\frac{(\text{SNR of } f_1)^2}{\text{number of transients}} = \left\langle \frac{s^2(t)}{\sigma_1^2(t)} \right\rangle,$$

which yields

$$\text{single-shot SNR of method 1} = \sqrt{\left\langle \frac{s^2(t)}{\sigma_1^2(t)} \right\rangle}. \tag{4.21}$$

In seeking a similar expression for f_2, consider an example in which $\sigma_1^2(t) = \sigma_2^2(t)$ and $Z_1 = Z_2$. The statistical information obtained using the two methods can be considered identical in this case, since each point is sampled the same number of times with the same distribution of noise. It follows that

$$\begin{aligned}(\text{SNR of } f_2)^2 &= (\text{SNR of } f_1)^2 \\ &= NZ_1 \frac{\langle s^2(t) \rangle}{\sigma_1^2} \\ &= NZ_2 \frac{\langle s^2(t) \rangle}{\sigma_2^2}.\end{aligned}$$

The "single-shot sensitivity" of method 2 is then found to be

$$\frac{(\text{SNR of } f_2)^2}{\text{number of transients}} = N \frac{\langle s^2(t) \rangle}{\sigma_2^2}.$$

The natural extension to the case of time-dependent noise would be

$$\text{single-shot SNR of method 2} = \sqrt{N \left\langle \frac{s^2(t)}{\sigma_2^2(t)} \right\rangle}. \tag{4.22}$$

These results can be written in a unified way as

$$SNR_{\text{real}} = \sqrt{QM \left\langle \frac{s^2(t)}{\sigma^2(t)} \right\rangle}, \tag{4.23}$$

where Q is the number of points sampled per transient, M is the total number of transients, and the average runs over all sampled points. We have included the subscript "real" as a reminder that the discussion has so far been limited to real-valued signals. In extending this definition to the case of a complex signal $s(t) = a(t) + ib(t)$, we adopt the point of view that in sampling the complex signal, we are seeking information about a real-valued function, such as the real component of a spectrum.

In addition, we assume that sampling a point of $a(t)$ or $b(t)$ contributes equally to the sensitivity with which we can measure this real-valued function. For the purpose of characterizing the sensitivity of the measurement, we consider the N sampled complex points equivalent to $2N$ sampled real points which measure a real-valued function. We can therefore define the SNR for a method which samples complex points by letting Q represent the total number of real points sampled per transient, and by letting the average inside the radical run over all sampled real points:

$$\begin{aligned} SNR_{\text{complex}} &= \sqrt{(QM)\frac{1}{2N}\sum\left(\frac{a^2(t)}{\sigma_a^2(t)}+\frac{b^2(t)}{\sigma_b^2(t)}\right)} \\ &= \sqrt{\frac{QM}{2}\left\langle\frac{a^2(t)}{\sigma_a^2(t)}+\frac{b^2(t)}{\sigma_b^2(t)}\right\rangle}. \end{aligned} \tag{4.24}$$

In (4.24), both the sum and the average are taken over the N sampled points of the complex function, and $\sigma_a^2(t)$, $\sigma_b^2(t)$ are the variances for respective measurements of $a(t)$, $b(t)$ without signal averaging.

3 Comparison with a standard definition

We wish to compare (4.24) with a standard definition given by Ernst in reference [20]. Consider first a nondecaying complex signal $s(t)$ which contains a single Fourier component that is sampled during a time period T:

$$s(t) = s_k e^{i\omega_k t}, \;\; 0 \le t \le T.$$

Normally-distributed, channel-independent white noise is assumed, which gives the measured values of $\mathrm{Re}\, s(t)$ and $\mathrm{Im}\, s(t)$ the same time-independent variance σ^2, and each transient is assumed to yield N sampled complex points. Since $Q = 2N$ and $|s(t)| = |s_k|$, we have

$$SNR = \frac{|s_k|}{\sigma/\sqrt{NM}}. \tag{4.25}$$

(To simplify notation, we have dropped the subscript "complex.") For a real spectrum containing one peak, Ernst defined the SNR as the ratio of peak height to root-mean-square noise in the real components of the spectrum [20]. In order to compare this definition with (4.25), we assume that the signal $s(t)$ is "properly phased," that is, we assume that s_k is real and positive. The peak height in our real spectrum is thus s_k. Let $x(n)$ represent the complex noise present in the n^{th} sampled point after averaging, and let the Fourier components of x be denoted by x_m. For each n, the mean value of $|x(n)|^2$ is $2\sigma^2/M$, since the real and imaginary parts of the noise have the same mean-square value σ^2/M after averaging. It follows that

$$\begin{aligned}\left\langle \sqrt{\frac{1}{N}\sum |x_m|^2} \right\rangle &= \left\langle \sqrt{\frac{1}{N^2}\sum |x(n)|^2} \right\rangle \\ &= \left\langle \sqrt{\frac{1}{N^2}\left(N\frac{2\sigma^2}{M}\right)} \right\rangle \\ &= \sqrt{2}\left(\sigma/\sqrt{NM}\right).\end{aligned}$$

We see that the root-mean-square noise in the real spectrum is $\sigma/\sqrt{NM}$, and that (4.25) can be written as

$$SNR = \frac{\text{peak height in real spectrum}}{\text{rms noise in real spectrum}}, \tag{4.26}$$

so that (4.24) agrees with Ernst's definition for this particular example.

We generalize the example by supposing that $s(t)$ is an arbitrary bounded complex signal which is sampled at N points within the interval $0 \leq t \leq T$. Assume as before that the noise in the measurement is white and independent of channel. In order to avoid introducing the unnecessary assumption that N complex points are sampled per transient, we define Z to be the number of averages performed in estimating each complex point of $s(t)$. The total number of real samples obtained during the measurement is

$$QM = 2NZ.$$

We have

$$SNR = \sqrt{ZN\left\langle \frac{a^2(t)+b^2(t)}{\sigma^2}\right\rangle} = \frac{\sqrt{\left\langle |s(t)|^2\right\rangle}}{\sigma/\sqrt{ZN}}. \tag{4.27}$$

Let s_k represent the k^{th} Fourier component of $s(t)$, and note that

$$\sqrt{\left\langle |s(t)|^2\right\rangle} = \sqrt{\frac{1}{N}\sum |s(t)|^2} = \sqrt{\sum |s_k|^2}.$$

With $x(n)$ and x_m defined as in the previous example, we find that the mean value of $|x(n)|^2$ is $2\sigma^2/Z$, and

$$\left\langle \sqrt{\frac{1}{N}\sum |x_m|^2}\right\rangle = \left\langle \sqrt{\frac{1}{N^2}\sum |x(n)|^2}\right\rangle = \left\langle \sqrt{\frac{1}{N^2}\left(N\frac{2\sigma^2}{Z}\right)}\right\rangle = \sqrt{2}\left(\sigma/\sqrt{NZ}\right).$$

The root-mean-square noise in the real spectrum is therefore $\sigma/\sqrt{ZN}$. It follows that

$$(SNR)^2 = \frac{\text{sum of all squared real and imaginary Fourier components of the signal}}{\text{mean-square noise in real spectral components}}. \tag{4.28}$$

Equation (4.28) highlights the difference between Ernst's definition of SNR and the one we have proposed. For this example, Ernst's definition could be obtained from (4.28) by discarding from the sum in the numerator the squares of all real and imaginary Fourier components with the exception of the largest real Fourier component.

We end this section by considering the limitations of our proposed definition. Note first that the SNR is determined once we know the total number of real-valued samples taken, and the average ratio

$$\langle R \rangle = \left\langle \frac{\text{signal magnitude squared}}{\text{variance in measured value}} \right\rangle,$$

where the average is taken over all real-valued samples. For any experiment being considered, the SNR we obtain will be the same as if we had made QM independent measurements of a single, real-valued random variable f for which the ratio

$$\frac{\text{mean value of } f}{\text{standard deviation of } f} = \sqrt{\langle R \rangle}.$$

This observation highlights a condition necessary for the validity of our definition: the noise in the QM real-valued samples must be statistically independent. If the noise in different sampled points is correlated (as in the case of spin noise during a single transient, for instance), then knowledge of these correlations could in general be used to increase the effectiveness with which information could be extracted from the measurement; that is, an analysis that takes account of the correlations should give a higher value of SNR than one which does not. In this case, we would expect our definition of SNR to underestimate the sensitivity of the measurement.

Another limitation of our definition is that it does not take account of the method we use in obtaining information from the spectrum; for instance, our definition of SNR does not specifically tell us how effectively we can obtain the frequency of a given peak in the spectrum. To highlight this point, we suppose that the signal $s(t)$ is a decaying exponential which will be sampled at intervals Δt during some time interval $0 \leq t \leq T$. How far toward zero should $s(t)$ be allowed to decay before the sampling is terminated? In seeking an optimal T, we begin by recalling the definition of the discrete Fourier transform s_k of a function $s(n)$ which is defined on a set of N

integers:

$$s(n) = \sum_k s_k \exp\{i(2\pi k/N)n\} \tag{4.29}$$

$$s_k = \frac{1}{N}\sum_n s(n)\exp\{-i(2\pi k/N)n\}. \tag{4.30}$$

Given a time T_0 such that $|s(t)|$ is close to zero for $t \geq T_0$, we can see from equation (4.30) that the height of each peak in the spectrum will be decreased by a factor of 2 if we sample during a period of length $2T_0$ rather than a period of length T_0. (Doubling the length of the sampling period doubles the value of N appearing in the denominator on the right side of (4.30), but it does not significantly change the value of the sum.) In the limit of large T, the height of each peak is proportional to $1/T$. The root-mean-square noise in the spectrum, however, does not decrease as quickly as the height of the spectrum, as can be seen from the relation

$$\frac{1}{N}\sum_n |x(n)|^2 = \sum_m |x_m|^2, \tag{4.31}$$

where $x(n)$ is the noise in the n^{th} sampled point, and x_m is a Fourier component. If the value of N is doubled, the left side of (4.31) does not change, while the number of Fourier components x_k is doubled. It follows that the root-mean-square noise in the spectrum, which can be written as

$$\text{rms spectral noise} = \sqrt{\frac{1}{N}\sum_m |x_m|^2},$$

varies as $1/\sqrt{T}$ in the limit of long T, and that the peak height becomes arbitrarily small in relation to the root-mean-square noise as $T \to \infty$.

Our definition of SNR claims that the sensitivity of the measurement does not change as T increases from T_0 toward infinity. This can be seen by noting that (4.27) gives

$$SNR = \frac{\sqrt{\langle |s(t)|^2 \rangle}}{\sigma / \sqrt{ZN}} = \frac{\sqrt{\sum |s(t)|^2}}{\sigma / \sqrt{Z}},$$

where the sum is over the N sampled points. Taking additional samples for which $|s(t)|^2 \approx 0$ does not affect the SNR.

To understand this property of our SNR definition, note that the ratio in (4.28) does not change as $T \to \infty$. Although the peak height becomes small relative to the root-mean-square noise, the sum of the signal's squared Fourier components does not become small relative to the mean-square noise. For long T, the statistical information about each peak is spread over a larger number of Fourier components separated by very small frequency increments. Although decreasing the peak height relative to the noise certainly makes the spectrum less pretty, it is not clear a priori whether a given method for extracting the position of a peak (for example) would be sensitive to the value of T, provided T is not pathologically long. To answer a question of this sort, it would be necessary to move beyond the general arguments we used in characterizing sensitivity and consider particular methods of extracting information from the spectrum.

4 Signal-to-noise ratio for amplitude detection

4.1 Definition of the signal

The BOOMERANG scheme for force-detected NMR spectroscopy [13, 21, 22] detects a single point of the free-induction decay (FID) for each measured transient. In this scheme, a conventional NMR pulse sequence is applied to the spins, and the spins precess freely for a period of time without being coupled to the resonator. At time t_1 during the FID, a transverse component $\langle I_x(t_1) \rangle$ is measured by using $\langle I_x(t_1) \rangle$ to drive the mechanical resonator. The driven spin component exerts a resonant driving force on the mechanical oscillator, and the resulting mechanical motion is detected. Analysis of the mechanical motion yields a measurement of $\langle I_x(t_1)\rangle$. By repeating the measurement for a range of values t_1, a record of the spins' time evolution is obtained, and Fourier analysis yields an NMR spectrum. This detection scheme is discussed in more detail in section 1 of chapter 5. In the current section, we derive a SNR formula for BOOMERANG detection in the case where the spin-resonator coupling has the form of equation (2.11).

In applying the SNR formula derived in section 1 to such detection schemes, we can define the signal $m(t)$ either in terms of the resonator's position coordinate or in terms of the torque exerted on the resonator by the spins. The analysis is simpler if the signal is defined as a torque, since the functional form of $m(t)$ is independent of the resonator's ringdown time τ_h. The driving torque is modulated by spin precession in the transverse plane, and it decays as $\langle I_x\rangle$ and $\langle I_y\rangle$ relax to zero. In obtaining a simple sensitivity estimate, we can consider the torque to be a single decaying sinusoid. However, the functional form of the resonator's response depends on the relative lengths of τ_h and the time period during which the torque is exerted. In general, $\langle\theta(t)\rangle$ will include an initial period of "ringing up," as well as a delayed response to changes in the amplitude of the driving torque, and so the functional form of $\langle\theta(t)\rangle$ will not always be well-approximated by a decaying sinusoid, even if the driving torque has that form. For sufficiently short τ_h, negligible error will be introduced by considering the resonator to be continually driven at steady-state, and since our analysis of resonator-induced spin relaxation assumed that τ_h is short compared to spin relaxation times, there is no inconsistency in analyzing sensitivity under the assumption of short τ_h. The assumption of short τ_h is unnecessary, however, and we can obtain more general results by defining the signal in terms of the torque exerted by the spins. (It should be pointed out that although it is convenient for purposes of sensitivity analysis to define the signal as a torque, it may not be the preferred method of analyzing experimental data. A practical protocol for data analysis would need to take account of the details of the experiment.)

For an experiment involving a macroscopic resonator and a large number of spins, the torque exerted by the spins is a clearly defined concept, since the resonator's evolution can be analyzed using classical mechanics, which includes explicit reference to forces and torques. In the current context, however, we are deriving SNR formulas which will be used to characterize the sensitivity of a low-temperature, high-frequency resonator interacting with a small spin sample, and so a quantum mechanical description is needed. In this context, an unproblematic definition of the torque can be made using the lab-frame master equation for the spin-resonator system:

$$\frac{d\rho}{dt} = -i\left[H_{\text{osc}} - \gamma \mathbf{I} \cdot \mathbf{B}\left(\theta\right), \rho\right] + \Lambda\rho, \tag{4.32}$$

where the relaxation superoperator Λ is given by (2.25). Evolution equations for the coordinate $\langle\theta\left(t\right)\rangle$ and the conjugate momentum $\langle p_\theta\left(t\right)\rangle$ can be obtained by multiplying equation (4.32) by θ and p_θ, respectively, and taking the trace:

$$\frac{d\langle\theta\rangle}{dt} = \frac{\langle p_\theta\rangle}{I_h} - \frac{\langle\theta\rangle}{\tau_h}, \tag{4.33}$$

$$\frac{d\langle p_\theta\rangle}{dt} = -k\langle\theta\rangle - \frac{\langle p_\theta\rangle}{\tau_h} + \left\langle \mu \cdot \frac{d}{d\theta}\mathbf{B}\left(\theta\right)\right\rangle, \tag{4.34}$$

where μ is the sample dipole. Note that in deriving the second equation, we used the identity

$$\left[p_\theta, F\left(\theta\right)\right] = -i\hbar\, dF/d\theta,$$

which follows from $[\theta, p_\theta] = i\hbar$. Equations (4.33) and (4.34) have the same form as the equations of motion for a classical torsional oscillator driven by a torque $\langle \mu \cdot \frac{d}{d\theta}\mathbf{B}\left(\theta\right)\rangle$, and we can consider this to be the torque exerted by the spins. Approximating $\mathbf{B}_h\left(\theta\right)$ by an expression first-order in θ as in section 1 of chapter 2 yields the simpler expression

$$m\left(t\right) = \gamma\hbar\frac{dB_x}{d\theta}\left\langle I_x\left(t\right)\right\rangle. \tag{4.35}$$

Equation (4.35) defines the signal which would be detected in a noiseless experiment.

In studying the sensitivity of NMR methods which detect $\langle I_x(t)\rangle$, we assume that

$$\langle I_x(t)\rangle = \begin{cases} \langle I_x(0)\rangle e^{-t/\tau_s}\cos\omega_h t & t \geq 0 \\ 0 & t < 0 \end{cases}. \tag{4.36}$$

Time $t = 0$ corresponds to the beginning of a detection period during which the mechanical oscillator experiences a resonant driving torque. The decay time of the transverse dipole during the detection period is denoted by τ_s. The signal can be expressed in the form

$$m(t) = Gm_0(t),$$

where

$$G = \gamma\hbar\frac{dB_x}{d\theta}\langle I_x(0)\rangle,$$

$$m_0(t) = \begin{cases} e^{-t/\tau_s}\cos\omega_h t & t \geq 0 \\ 0 & t < 0 \end{cases}. \tag{4.37}$$

The method developed in section 1 will be used to estimate the sensitivity with which G can be measured.

4.2 Definition of the noise

Equations (4.3) and (4.4) of section 1 give the SNR of the amplitude estimate X as

$$SNR = \frac{\langle G\rangle}{\sqrt{\sigma_G^2 + \sigma_{\text{noise}}^2}}.$$

Note first that since

$$G = \gamma\hbar\frac{dB_x}{d\theta}\langle I_x(0)\rangle \tag{4.38}$$

is an ensemble average, it has a definite value, rather than being a random variable, and so

$$\sigma_G^2 = 0.$$

The variance of X is equal to σ^2_{noise}, which can be calculated if the spectral density $S_n(\omega)$ of the noise is known.

In deriving an expression for $S_n(\omega)$, we begin by defining the noisy signal $f(t) = m(t) + n(t)$. Continuous observation of the resonator yields a measured coordinate $\theta_{\text{obs}}(t)$. Given $\theta_{\text{obs}}(t)$, in addition to measured values of I_h, ω_h, and τ_h, equations (4.33) and (4.34) can be used to calculate the driving torque which would cause the expected value of the resonator's coordinate to equal $\theta_{\text{obs}}(t)$. This calculated driving torque is the noisy signal $f(t)$. Equivalently, the noise $n(t)$ can be defined as the torque which would produce mean displacement $\delta\theta_{\text{obs}}(t)$ in the resonator, where $\delta\theta_{\text{obs}}(t)$ is given by

$$\delta\theta_{\text{obs}}(t) = \theta_{\text{obs}}(t) - \langle\theta(t)\rangle\,,$$

and the average $\langle\theta(t)\rangle$ is taken over an ensemble of spin-resonator systems.

Spin fluctuations and the thermal fluctuations in θ are two intrinsic noise sources. In addition, quantum mechanics imposes limitations on the sensitivity with which motion can be detected. Section 4.3 presents formulas for the spectral density of the noise introduced by thermal fluctuations in θ and the noise introduced by the motion detector. Section 4.4 derives an expression for the spectral density of the spin noise.

4.3 Spectral density of the instrument noise

The evolution of the Heisenberg operator $\theta(t)$ is given to first order in θ by the quantum Langevin equation

$$I_h \frac{d^2}{dt^2}\theta(t) + \frac{2I_h}{\tau_h}\frac{d}{dt}\theta(t) + k\theta(t) = \gamma\hbar\frac{dB_x}{d\theta}I_x(t) + N'(t)\,, \tag{4.39}$$

where $N'(t)$ is a fluctuating thermal torque. The quantum Langevin equation for a damped resonator is derived in reference [23], and a similar derivation can be carried out when $\theta(t)$ is coupled to $I_x(t)$. Equation (4.39) shows that the intrinsic fluctuations θ for the spin-resonator system can be characterized in terms of a thermal torque. The spectral distribution of the thermal torque is calculated using the symmetric correlation function

$$C_{N'}(t_1,t) = \frac{1}{2}\left\langle N'(t)\,N'(t_1) + N'(t_1)\,N'(t)\right\rangle,$$

which can be expressed as [23]

$$C_{N'}(t_1,t) = \frac{2I_h}{\tau_h}\frac{1}{\pi}\int_0^{\infty}\hbar\omega\coth\left(\frac{\hbar\omega}{2k_BT_h}\right)\cos\left[\omega\left(t-t_1\right)\right]\,d\omega. \tag{4.40}$$

Equation 4.40 implies that the double-sided spectral density $S_{N'}(\omega)$ of $N'(t)$ is given by

$$S_{N'}(\omega) = \frac{4I_h}{\tau_h}\hbar\omega\left(\frac{1}{2} + n_{\text{th}}(\omega)\right),\ \omega \geq 0, \tag{4.41}$$

where $n_{\text{th}}(\omega)$ is the number of thermal quanta in an oscillator of frequency ω at temperature T_h. (Since a double-sided spectral density is an even function of ω, it suffices to specify its values for $\omega \geq 0$.)

If $\hbar\omega_h \ll k_BT_h$, then (4.41) is closely approximated by the classical expression

$$S_{N'}(\omega) = \frac{4I_hk_BT_h}{\tau_h}.$$

At frequencies of order 50 MHz or higher and temperatures of order 10 mK, which are achievable in a dilution refrigerator, mechanical zero-point motion makes a non-negligible contribution to the intrinsic fluctuations characterized by (4.41), since $n_{\text{th}}(\omega_h)$ is of order unity or less. In this regime, quantum mechanics imposes limitations on the sensitivity with which $\langle\theta(t)\rangle$ can be measured. In the limit where the temperature approaches zero Kelvins, the spectral density of the thermal torque is

$$S_{N'}(\omega,0) = \frac{4I_h}{\tau_h}\hbar\omega\left(\frac{1}{2}\right).$$

Quantum-limited detection of the oscillator's motion occurs when the noise added by the detector is equivalent to the noise resulting from the thermal torque at zero Kelvins [24]. Letting $S_{\text{QL}}(\omega)$ denote the spectral density of the quantum-limited "noise torque," which includes contributions from the thermal torque as well as the noise added by the detector, we have

$$S_{\mathrm{QL}}(\omega) = \frac{4I_h}{\tau_h}\hbar\omega\left(\frac{1}{2} + \frac{1}{2} + n_{\mathrm{th}}(\omega)\right), \ \omega \geq 0.$$

The nature of this quantum limit is clarified by remarks presented in references [11] and [24]. Achievement of quantum-limited detection sensitivity requires that the strength of the coupling between oscillator and detector be optimally tuned. For overly weak coupling, the detector's response to the mechanical motion becomes small compared to the detector's intrinsic fluctuations, while for overly strong coupling, the "back-action," or perturbation of the mechanical oscillator due to its coupling to the detector, becomes large relative to the intrinsic mechanical fluctuations characterized by $S_{N'}(\omega)$ [24]. The minimal noise added to the signal by an optimal detection scheme can be interpreted as the zero-point motion of an internal mode of the detector [11].

In characterizing the performance of a real detector, we let $S_{\mathrm{inst}}(\omega)$ denote the spectral density of "instrument noise," that is, the noise not present in the spin sample itself, and we assume that $S_{\mathrm{inst}}(\omega)$ can be expressed in the form

$$S_{\mathrm{inst}}(\omega) = \frac{4I_h}{\tau_h}\hbar\omega\left(A_{\mathrm{det}} + \frac{1}{2} + n_{\mathrm{th}}(\omega)\right), \ \omega \geq 0. \tag{4.42}$$

(In practice, this will be equivalent to the assumption that the detector adds white noise, since $S_{\mathrm{inst}}(\omega)$ is flat in the bandwidth of interest for NMR signals.) We could say that in this case the noise added by the resonator is $2A_{\mathrm{det}}$ times the quantum limit. More conventional (but less straightforward) is the use of noise temperature T_N, for which different authors give inconsistent definitions [11, 24]. A simple approach might be to define T_N by the equation

$$A_{\mathrm{det}} + \frac{1}{2} + n_{\mathrm{th}}(\omega_h, T_h) = \frac{1}{2} + n_{\mathrm{th}}(\omega_h, T_h + T_N), \tag{4.43}$$

or

$$A_{\mathrm{det}} = n_{\mathrm{th}}(\omega_h, T_h + T_N) - n_{\mathrm{th}}(\omega_h, T_h),$$

where A_{det} is defined as in (4.42), and where the temperature dependence of n_{th} has been highlighted by expressing its argument as (ω_h, T_h). From (4.43) we see that the noise temperature can be roughly interpreted as the increase in resonator temperature needed to account for the noise added by the detector. A weakness of this definition is that the detector's noise temperature depends on the amount of noise at the input (i.e., the temperature of the resonator), which implies that noise temperature does not characterize the "intrinsic" properties of the detector. Differing attempts to correct this weakness lead to inconsistent definitions of noise temperature.

We follow reference [25] in defining the quantum-limited noise temperature T_{QL} by

$$T_{QL} = \frac{\hbar\omega_h}{k_B \ln 3}. \tag{4.44}$$

Equation (4.44) is obtained by defining the noise temperature T_N in reference to an oscillator at 0 K, so that

$$A_{\text{det}} = n_{\text{th}}\left(\omega_h, T_N\right).$$

Schwab et al. have reported detection of mechanical motion with [25]

$$T_N = 18 T_{QL},$$

which gives

$$A_{\text{det}} = 16. \tag{4.45}$$

In adding noise to simulations of detected spectra in section 1 of chapter 6, we assume that the detector has this value of A_{det}, so that the "noise torque" associated with thermal fluctuations and detector noise has spectral density

$$S_{\text{inst}}\left(\omega\right) = \frac{4I_h}{\tau_h}\hbar\omega\left(16 + \frac{1}{2} + n_{\text{th}}\left(\omega\right)\right), \;\; T_N = 18T_{QL}, \, \omega \geq 0.$$

4.4 Spectral density of the spin noise

Superimposed on $m(t)$ is a noise torque $T'(t)$ associated with fluctuations of $I_x(t)$. In quantifying these fluctuations, we use a simple model in which they are treated as a stationary random process with zero mean during the period in which the resonator's position is being monitored. The properties of this random process are calculated using a high-temperature limit, without consideration of the pulse sequence used during the NMR experiment. In certain cases, this model could overestimate the spin noise. Consider, for instance, an experiment in which the longitudinal magnetization of a highly-polarized sample is rotated by 90° to lie along the x-axis at the beginning of the detection period. The variance in I_x at the beginning of the detection period is then equal to the variance in I_z just before the rotation. If the spin sample is at a temperature of $\sim$ 10 mK and is in an applied field of order 10 T, the variance in I_z is significantly less than the high-temperature limit, and the spin noise could be overestimated as a result.

The spectral distribution of the spin noise can be quantified by means of the symmetric correlation function

$$C_I(t_1, t) = \frac{1}{2}\langle I_x(t)\, I_x(t_1) + I_x(t_1)\, I_x(t)\rangle .$$

Use of the quantum regression theorem [7] in combination with equation (4.36) gives

$$C_I(t_1, t) = \left\langle I_x^2 \right\rangle e^{-|t-t_1|/\tau_s} \cos\left(\omega_h |t - t_1|\right) .$$

Note that the value of the time constant τ_s for decay of the transverse spin dipole will depend on whether the spins precess freely or are spin-locked. For the mean-square fluctuation $\langle I_x^2\rangle$ we use the value $N/4$, appropriate for a sample of N spins 1/2 in thermal equilibrium. The symmetric correlation of the spin-noise torque $T'(t)$ is in this way approximated as

$$C_{T'}(t_1,t) = \frac{1}{2}\langle T'(t)\,T'(t_1) + T'(t_1)\,T'(t)\rangle$$
$$= \left(\gamma\hbar\frac{dB_x}{d\theta}\right)^2 \frac{N}{4} e^{-|t-t_1|/\tau_s}\cos\left(\omega_h\,|t-t_1|\right),$$

and the spectral density $S_{T'}(\omega)$ as

$$S_{T'}(\omega) = \left(\gamma\hbar\frac{dB_x}{d\theta}\right)^2 \frac{N}{4}\int_{-\infty}^{\infty} e^{-i\omega t} e^{-|t|/\tau_s}\cos\left(\omega_h t\right) dt. \tag{4.46}$$

4.5 SNR formula for amplitude detection

In order to simplify the analysis, we will calculate SNR using a filter which is optimal if spin noise is negligible compared to the thermal torque $N'(t)$ and the detector noise. The transfer function $K(\omega)$ is

$$K(\omega) = c\frac{M_0^*(\omega)}{S_{\mathrm{inst}}(\omega)},$$

where $S_{\mathrm{inst}}(\omega)$ is given by equation (4.42), and $M_0(\omega)$ is the Fourier transform of the unit amplitude signal defined by (4.37). The curve $M_0(\omega)$ has complex Lorentzian peaks at $\pm\omega_h$. The magnitude of S_{inst} varies by at most a few percent over the range of frequencies for which $M_0(\omega)$ is non-negligible, assuming that $\omega_h/2\pi$ is in the range of 50 MHz to 1 GHz, with

$$T_h \geq 10\ \mathrm{mK},$$
$$\tau_s \geq 1\,\mu\mathrm{s},$$
$$A_{\mathrm{det}} \leq 10^3.$$

We will therefore approximate $S_{\mathrm{inst}}(\omega)$ by $S_{\mathrm{inst}}(\omega_h)$ and consider the noise to be white. The constant c is chosen as in equation 4.13:

$$c = S_{\mathrm{inst}}(\omega_h).$$

When the noisy signal $f(t) = m(t) + n(t)$ is passed into filter $\mathcal{K}$, the output $\phi(t) = \mu(t) + \nu(t)$ is given by equation (4.14) as

$$\phi(t) = \int_{-\infty}^{\infty} f(t') \, m_0(t' - t) \, dt'.$$

The amplitude estimate X is given by equations (4.15) and (4.17):

$$X = \frac{\int_{-\infty}^{\infty} m_0(t) \, f(t) \, dt}{\int_{-\infty}^{\infty} m_0^2(t) \, dt}.$$

The SNR formula (4.7) can be expressed as

$$SNR = \frac{\langle X \rangle}{\sqrt{\sigma_{\text{inst}}^2 + \sigma_{\text{spin}}^2}},$$

where σ_{inst}^2, σ_{spin}^2 are the respective variances introduced into the measurement by instrument noise and spin noise:

$$\sigma_{\text{inst}}^2 = \frac{1}{\mu_0^2} \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} |M_0(\omega)|^2 \, S_{\text{inst}}(\omega) \, d\omega \right), \tag{4.47}$$

$$\sigma_{\text{spin}}^2 = \frac{1}{\mu_0^2} \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} |M_0(\omega)|^2 \, S_{T'}(\omega) \, d\omega \right), \tag{4.48}$$

$$\mu_0 = \int_{-\infty}^{\infty} m_0^2(t) \, dt \approx \frac{\tau_s}{4}.$$

Evaluation of the integrals appearing in (4.47) and (4.48) yields

$$\sigma_{\text{inst}}^2 = S_{\text{inst}}(\omega_h) \frac{4}{\tau_s},$$

$$\sigma_{\text{spin}}^2 = \frac{N}{2} \left(\gamma \hbar \frac{dB_x}{d\theta} \right)^2.$$

The mean value $\langle X \rangle = G$ is given by equation (4.38):

$$\langle X \rangle = \gamma \hbar \frac{dB_x}{d\theta} \langle I_x \rangle.$$

Here $\langle I_x \rangle$ is a mean transverse spin component at the beginning of the time period during which the torque on the mechanical resonator has the form of a decaying sinusoid. The value of $\langle I_x \rangle$ depends on the sequences of pulses and delays used to encode information about the microscopic environment of the spins into the motion of the transverse spin dipole. For the SNR estimate, we assume that the value of $\langle I_x \rangle$ at the beginning of the FID is $PN/2$, where P is the polarization of the spin sample just before the beginning of the pulse sequence. The time-dependence of $\langle I_x \rangle$ during the sampled portion of the FID is characterized by the function $s_0(t)$, which is defined by the equation

$$\langle I_x(t_1) \rangle = \frac{PN}{2} s_0(t_1) . \tag{4.49}$$

To characterize the sensitivity of a single measurement of $\langle I_x \rangle$ as a means of detecting the FID, we use equation (4.21), which can be expressed in this case as

$$\text{single-shot SNR} = \frac{(PN/2)\sqrt{\langle s_0^2(t_1) \rangle}}{\sqrt{\sigma_{\text{inst}}^2 + \sigma_{\text{spin}}^2}} .$$

The single-shot SNR for detection of an FID by measurement of an amplitude $\langle I_x \rangle$ is

$$\begin{aligned} \text{single-shot } SNR &= \frac{(PN/2)(\gamma\hbar\, dB_x/d\theta)\sqrt{\langle s_0^2(t_1) \rangle}}{\sqrt{S_{\text{inst}}(\omega_h)(4/\tau_s) + (N/2)(\gamma\hbar\, dB_x/d\theta)^2}}, \\ S_{\text{inst}}(\omega_h) &= \frac{4I_h}{\tau_h}\hbar\omega_h\left(A_{\text{det}} + \frac{1}{2} + n_{\text{th}}(\omega_h)\right) . \end{aligned} \tag{4.50}$$

Note that the spectral density $S_{\text{inst}}(\omega_h)$ is a double-sided spectral density. Equation (4.50) could be expressed in terms of a single-sided spectral density $S_{\text{inst}}^{\text{s}}(\omega_h)$ by making the substitution $S_{\text{inst}}(\omega_h) = S_{\text{inst}}^{\text{s}}(\omega_h)/2$.

If the amplitude measurement is performed by spin-locking the transverse spin dipole, with resonator-induced relaxation responsible for decay of the spin-locked signal, then the results of section 6 of chapter 3 imply that

$$\tau_s = 2/R_h,$$

provided the spin-locking field is strong enough to average both the internal spin Hamiltonian and the spin relaxation superoperator associated with spin-resonator interactions. If, in addition, instrument noise is much larger than spin noise, then (4.50) can be simplified to yield

$$\begin{aligned}\text{single-shot } SNR &= \frac{(PN/2)\left(\gamma\hbar\, dB_x/d\theta\right)\sqrt{\left\langle s_0^2\left(t_1\right)\right\rangle}}{\sqrt{S_{\text{inst}}\left(\omega_h\right)\left(2R_h/\tau_s\right)}} \\ &= \frac{PN\sqrt{\left\langle s_0^2\left(t_1\right)\right\rangle}}{4\sqrt{\left(A_{\text{det}}+\frac{1}{2}+n_{\text{th}}\right)\left(n_{\text{th}}+\frac{1}{2}\right)}}. \end{aligned} \tag{4.51}$$

In this case, the SNR is independent of the resonator parameters τ_h, I_h, and $dB_x/d\theta$. We can interpret (4.51) as stating that if the resonator ringdown time, moment of inertia, and field derivative $dB_x/d\theta$ are considered to be "knobs" which can be varied, then changes in transverse relaxation due to lifetime broadening will compensate exactly for changes in the signal strength and the Brownian noise as these knobs are turned. The only resonator parameter which appears in the SNR expression is the thermal number of quanta n_{th}, which is determined by the resonator frequency ω_h and the temperature T_h.

5 Signal-to-noise ratio for detection of a continuous signal

If the freely-precessing transverse spin dipole drives the resonator throughout the FID, then detection of a single transient yields a measurement of the time-dependent function $\langle I_x(t)\rangle$ rather than a single amplitude $\langle I_x(t_1)\rangle$. In characterizing the sensitivity of this method, we assume that a sampling interval Δt has been chosen, and that broadband noise with spectral density $S_{\text{inst}}(\omega_h)$ is present in the measurement, with $S_{\text{inst}}(\omega_h)$ given by equation (4.42). This noise is filtered before the noisy signal is sampled, and we assume for the sake of simplicity that an ideal bandpass filter eliminates all noise outside a frequency range of width $(1/\Delta t)$ Hz, and that the filtered noise introduces an identical variance σ^2 to each real-valued sample.

The definitions of the signal and the noise are similar to those given in sections 4.1 and 4.2. The signal $s(t)$ is defined as the torque which would produce mean displacement $\langle \theta(t) \rangle$ in the resonator, where the average is quantum statistical. Noise is present in the measurement due to the fact that

$$\theta_{\text{obs}}(t) \neq \langle \theta(t) \rangle ,$$

with $\theta_{\text{obs}}(t)$ the observed displacement. The noisy signal $f(t)$ is defined as the torque needed to produce a mean displacement equal to $\theta_{\text{obs}}(t)$, and the noise $n(t)$ is given by

$$n(t) = f(t) - s(t) .$$

Detection of a single transient yields a measurement of the driving torque exerted by the spins throughout the FID, and the signals from two transients can be combined to yield a complex signal, as in conventional NMR spectrometers. We will consider $s(t)$ to be complex, with two transients required to sample the full curve $s(t)$.

Using equation (4.27), the signal-to-noise ratio can be expressed as

$$SNR = \frac{\sqrt{\sum |s(t)|^2}}{\sigma/\sqrt{Z}},$$

where the sum is over the sampled complex points, with each point sampled Z times. We assume that the sampling interval is so short compared to the decay time of $|s(t)|^2$ that the average appearing underneath the radical can be approximated as an integral:

$$\begin{aligned}\sum |s(t)|^2 &= \frac{1}{\Delta t} \sum |s(t)|^2 \Delta t \\ &\approx \frac{1}{\Delta t} \int_0^\infty |s(t)|^2 \, dt \\ &\equiv \frac{1}{\Delta t} \left\langle |s(t)|^2 \right\rangle .\end{aligned}$$

We obtain

$$SNR \approx \frac{\sqrt{\left\langle |s\,(t)|^2 \right\rangle}}{\sqrt{\sigma^2 \Delta t / Z}}. \tag{4.52}$$

In the case where instrument noise is the dominant noise source, the variance introduced by this noise in a bandwidth of $(1/\Delta t)$ Hz is

$$\sigma^2 = \frac{S_{\text{inst}}\,(\omega_h)}{\Delta t}. \tag{4.53}$$

Substituting this expression into (4.52) and noting that $2Z$ transients were observed yields

$$\text{single-shot } SNR \approx \frac{\sqrt{\left\langle |s\,(t)|^2 \right\rangle}}{\sqrt{2 S_{\text{inst}}\,(\omega_h)}}. \tag{4.54}$$

For convenience in comparing the sensitivity of different detection schemes, we express $s\,(t)$ in the form

$$s\,(t) = \left(\frac{PN}{2}\right)\left(\gamma\hbar \frac{dB_x}{d\theta}\right)\{s_a\,(t) + i\, s_b\,(t)\}\,. \tag{4.55}$$

If

$$\begin{aligned} \left\langle |s_a\,(t) + i\, s_b\,(t)|^2 \right\rangle &= \left\langle s_a^2\,(t) \right\rangle + \left\langle\, s_b^2\,(t) \right\rangle \\ &= 2\left\langle s_a^2\,(t) \right\rangle, \end{aligned}$$

then (4.54) can be written as

$$\text{single-shot } SNR \approx \frac{(PN/2)\,(\gamma\hbar\, dB_x/d\theta)\,\sqrt{\langle s_a^2\,(t)\rangle}}{\sqrt{S_{\text{inst}}\,(\omega_h)}}. \tag{4.56}$$

6 Comparison of detection sensitivities

6.1 Dependence of sensitivity on the energy in the signal

The signal-to-noise ratios given in equations (4.50) and (4.56) can be compared in the case where instrument noise is dominant in (4.50). Dropping spin noise from (4.50) and taking the ratio of the two expressions gives

$$\left(\frac{\text{single-shot } SNR \text{ amplitude detection}}{\text{single-shot } SNR \text{ continuous signal}}\right)^2 = \frac{\left\langle s_0^2\left(t_1\right)\right\rangle}{\left(4/\tau_s\right)\left\langle s_a^2\left(t\right)\right\rangle} = \frac{\left\langle s_0^2\left(t_1\right)\right\rangle \left\langle m_0^2\left(t\right)\right\rangle}{\left\langle s_a^2\left(t\right)\right\rangle}. \tag{4.57}$$

Note that $\left\langle s_0^2\left(t_1\right)\right\rangle$ is an average over a set of times t_1 at which spin-locking was applied to obtain an amplitude measurement, and the signal s_0 corresponds to free spin precession in the absence of spin-resonator interaction. By way of contrast, the signal s_a appearing in the denominator of (4.57) corresponds to free spin precession in the presence of coupling to a mechanical resonator. Equation (4.57) can be interpreted as the ratio of the mean energies in the signals which drive the resonator in the two types of detection, with the average being taken over all transients. During continuous detection, the energy in the signal torque is proportional to $\left\langle s_a^2\left(t\right)\right\rangle$, while during an amplitude measurement, the resonator is driven by a signal torque proportional to $m_0\left(t\right)$ and having energy proportional to $\left\langle m_0^2\left(t\right)\right\rangle$. The proportionality constant for the spin-locked signal depends on the value of

$$\left\langle I_x\left(t_1\right)\right\rangle \propto s_0\left(t_1\right),$$

and the average $\left\langle s_0^2\left(t_1\right)\right\rangle$ includes the effect of this variation on detection sensitivity.

To further clarify the content of (4.57), we consider an example in which $s\left(t\right)$ has the form of a single decaying exponential with time constant T_2:

$$s\left(t\right) = \left(\frac{PN}{2}\right)\left(\gamma\hbar\frac{dB_x}{d\theta}\right)\exp\left\{\left(i\omega_0 - 1/T_2\right)t\right\}, \;\; t \geq 0,$$

with the time constant τ_s for the decay of $m_0\left(t\right)$ given by $T_{1\rho}$, the time constant for the decay of a spin-locked signal:

$$\tau_s = T_{1\rho}.$$

During amplitude measurements, the value of $\left\langle I_x\left(t_1\right)\right\rangle$ is sampled only at times t_1 when the FID has not decayed significantly. For this example, the ratio of equation

(4.57) can be expressed as

$$\left(\frac{\text{single-shot } SNR \text{ amplitude detection}}{\text{single-shot } SNR \text{ continuous signal}}\right)^2 = \frac{T_{1\rho}/2}{T_2}. \tag{4.58}$$

The factor of 2 difference arises from the fact that the initial amplitude of the signal for continuous detection does not vary between measurements, while the initial signal amplitude for spin-locked detection varies sinusoidally as t_1 is varied between shots.

6.2 Effect of resonator-induced transverse relaxation

Equations (4.57) and (4.58) show that the relative sensitivities of spin-locked detection and detection of freely-precessing spins are determined by the time constants for decay of the transverse spin. At mK temperatures, the precessing transverse spin of a solid sample containing only a few spins (e.g., two or three spins) is expected to relax slowly in the absence of spin-resonator interactions, since in this case transverse relaxation depends on spin-lattice interactions which are "frozen out" at low temperatures. The coupling between the spins and the mechanical resonator will induce transverse relaxation, thereby limiting the sensitivity with which the spectrum can be detected. Consider an example in which the sample contains only a single spin 1/2 and the resonator is at zero Kelvins. If interaction with the mechanical resonator is the dominant source of transverse relaxation, then it follows from equations (2.22) and (2.23) that the time constant for transverse relaxation is $2/R_h$. The signal $s(t)$ which drives the resonator is

$$s(t) = \left(\frac{P}{2}\right)\left(\gamma\hbar\frac{dB_x}{d\theta}\right)\exp\left\{(i\omega_0 - R_h/2)\,t\right\}, \quad t \geq 0,$$

and the single-shot SNR given by (4.56) evaluates to

$$\text{single-shot } SNR = \frac{P}{4\sqrt{\left(n_{\text{th}} + \frac{1}{2}\right)\left(n_{\text{th}} + \frac{1}{2} + A_{\text{det}}\right)}}, \quad \text{(free precession).} \tag{4.59}$$

Equation (4.59) can be compared with the sensitivity for spin-locked detection given by (4.51):

$$\text{single-shot } SNR = \frac{PN\sqrt{\langle s_0^2\left(t_1\right)\rangle}}{4\sqrt{\left(n_{\text{th}}+\frac{1}{2}\right)\left(A_{\text{det}}+\frac{1}{2}+n_{\text{th}}\right)}},\quad \text{(spin locking)},$$

where $N = 1$ and

$$s_0\left(t_1\right) = \cos\left(\omega_0 t_1\right).$$

Note that since the spins and the resonator are out of resonance until the spin-locking field is applied, the resonator is assumed not to induce transverse relaxation before spin-locking begins, and so negligible decay in $s_0\left(t_1\right)$ is also assumed. Since

$$\sqrt{\langle s_0^2\left(t_1\right)\rangle} = \frac{1}{\sqrt{2}},$$

we have

$$\frac{\text{single-shot } SNR \text{ free precession}}{\text{single-shot } SNR \text{ spin locking}} = \sqrt{2}. \tag{4.60}$$

Equation (4.60) is consistent with (4.58), since our assumptions have yielded

$$T_{1\rho} = T_2 = 2/R_h.$$

We next consider examples of two-spin systems in which a 90° pulse applied to a system in thermal equilibrium leaves the mean dipole aligned with the x-axis. For simplicity, the resonator is assumed to be at zero Kelvins. For a two-spin system in which the dipolar couplings are large compared to the difference in the chemical shift at the two spins, the energy eigenstates can be approximated as

$$\begin{aligned}
|p\rangle &\equiv |{+}{+}\rangle, \\
|q\rangle &\equiv \left(|{+}{-}\rangle + |{-}{+}\rangle\right)/\sqrt{2}, \\
|r\rangle &\equiv |{-}{-}\rangle, \\
|s\rangle &\equiv \left(|{+}{-}\rangle - |{-}{+}\rangle\right)/\sqrt{2}.
\end{aligned}$$

It follows from equation (3.33) that if the resonator is at zero Kelvins, the signal $s(t)$ driving the resonator during detection of freely precessing spins can be written as

$$\begin{aligned} s(t)/G &= \frac{1}{2}\exp\{(i\omega_{pq} - 1/T_{pq})\,t\} + \frac{1}{2}\exp\{(i\omega_{qr} - 1/T_{qr})\,t\}, \quad t \geq 0, \qquad (4.61) \\ T_{pq}^{-1} &= R_0, \\ T_{qr}^{-1} &= 2R_0. \end{aligned}$$

If the peaks associated with these two coherences do not overlap appreciably, then

$$\frac{1}{G^2}\int_0^\infty |s(t)|^2\,dt \approx \frac{(T_{pq} + T_{qr})/2}{4}. \qquad (4.62)$$

Note that for a signal $s(t)$ which has two frequency components decaying exponentially with arbitrary time constant T', we have

$$\frac{1}{G^2}\int_0^\infty |s(t)|^2\,dt = \frac{T'}{4}, \qquad (4.63)$$

provided that the frequency difference between the two components is much greater than $1/T'$. Comparing (4.62) and (4.63), we see that the effective decay time associated with (4.61) is

$$\begin{aligned} T_{\mathrm{eff,dd}} &= (T_{pq} + T_{qr})/2 \\ &= \frac{3}{4R_0}. \end{aligned}$$

By comparing this with the time constant $2/R_0$ for a single-spin system, we see that the decay time has decreased by 3/8. In the case where the chemical shift offset of one spin is much larger than the dipolar coupling, equation (3.34) can be used to obtain a similar result. The effective time constant is

$$\begin{aligned} T_{\mathrm{eff,dd+shift}} &= \left(\frac{2}{R_0} + \frac{2}{3R_0}\right)/2 \\ &= \frac{4}{3R_0}, \end{aligned}$$

which is smaller than $2/R_0$ by a factor of $2/3$.

These examples have shown that resonator-induced transverse relaxation can make a nonnegligible change in signal lifetime as the sample size is increased from $N = 1$ to $N = 2$. Simulations of resonator-induced transverse relaxation in four-spin systems are presented in section 2.2 of chapter 6, and those simulations suggest that the effective decay time of a freely-precessing signal decreases sharply as the number of dipole-dipole coupled spins is increased above two. By way of contrast, the decay time of the spin-locked signal does not depend on the size of the sample, provided the spin-locking field is strong enough to average both the internal Hamiltonian and the superoperator for resonator-induced relaxation. Ideal spin-locked detection is more sensitive than detection of free precession, even in the case of the two spin sample having $T_{\text{eff,dd}} = 3/(4R_0)$:

$$\begin{aligned}\frac{\text{single-shot } SNR \text{ free precession}}{\text{single-shot } SNR \text{ spin locking}} &= \sqrt{2}\sqrt{3/8} \\ &= \sqrt{3/4}.\end{aligned}$$

As sample size is increased, we may expect that detection of free precession will be substantially less sensitive than spin-locked detection, even if the number of spins is small enough that spin locking would not be needed to extend the lifetime of the signal in the absence of resonator-induced relaxation.

7 Dependence of signal-to-noise ratio and acquisition time on resonator parameters

In the case where instrument noise is dominant and the spin-locked signal decays exponentially with rate constant $R_h/2$, the single-shot SNR is given by (4.51) as

$$\text{single-shot } SNR = \frac{PN\sqrt{\langle s_0^2(t_1)\rangle}}{4\sqrt{\left(A_{\text{det}} + \frac{1}{2} + n_{\text{th}}\right)\left(n_{\text{th}} + \frac{1}{2}\right)}}.$$

Given a sample of N spins and a pulse sequence which yields signal $s_0(t_1)$, the dependence of SNR on resonator parameters can be expressed as

$$\text{single-shot } SNR \propto \frac{P}{\sqrt{\left(A_{\text{det}}+\frac{1}{2}+n_{\text{th}}\right)\left(n_{\text{th}}+\frac{1}{2}\right)}}, \tag{4.64}$$

$$P = \tanh\left(\frac{\hbar\omega_h}{2k_B T_h}\right),$$

$$n_{\text{th}} = \left(\exp\left(\frac{\hbar\omega_h}{k_B T_h}\right)-1\right)^{-1}.$$

The only resonator parameter which contributes to P and n_{th} is the ratio ω_h/T_h of frequency to temperature. If this ratio is increased, polarization increases and n_{th} decreases, and both of these changes improve SNR. In general, therefore, sensitivity improves when the frequency increases or the temperature decreases. However, the limiting values of P and n_{th} in the high-frequency, low-temperature limit are

$$P \to 1,$$

$$n_{\text{th}} \to 0.$$

For the example resonator presented in chapter 5, the values

$$T_h = 10 \text{ mK}, \tag{4.65}$$

$$\omega_h/2\pi = 630\,\text{MHz} \tag{4.66}$$

give

$$P = 0.91,$$

$$n_{\text{th}} = 0.05.$$

In this regime, SNR is near the value high-frequency, low-temperature limit.

Decreasing the ω_h/T_h by a factor of three (e.g., by increasing T_h to 30 mK) gives

$$P = 0.46,$$
$$n_{\text{th}} = 0.6.$$

In the case where the noise added by the motion detector is substantially larger than the noise associated with the zero-point motion of the resonator ($A_{\text{det}} \gg 1/2$), this change in ω_h/T_h decreases the right side of (4.64) by a factor of approximately 2.8. We see that although the regime defined by (4.65) and (4.66) is near optimal, SNR is sensitive to changes in ω_h/T_h within this regime.

The time required to acquire a spectrum is more sensitive to resonator parameters than the SNR is. Consider a problem in which the time needed per transient is proportional to $1/R_h$; for example, a problem in which both the decay of the spin-locked signal and the longitudinal relaxation occur during a time proportional to $1/R_h$, with the pulse sequence requiring a negligible period of time per transient. Since the number of transients Z needed to detect $\langle I_x(t_1)\rangle$ with acceptable accuracy at a given point t_1 is proportional to $1/(SNR)^2$, acquisition time is minimized if the resonator is designed to yield a minimal value of

$$\frac{1}{R_h (SNR)^2}$$

or, equivalently, a maximal value of

$$\begin{aligned}(SNR)^2 R_h &\propto \frac{P^2}{\left(A_{\text{det}} + \frac{1}{2} + n_{\text{th}}\right)} g^2 \tau_h \\ &\propto \frac{P^2}{\omega_h \left(A_{\text{det}} + \frac{1}{2} + n_{\text{th}}\right)} \frac{(dB_x/d\theta)^2}{I_h} \tau_h. \end{aligned} \tag{4.67}$$

The dependence of τ_h on other resonator parameters is poorly understood. If this dependence is neglected, then (4.67) can be used to analyze the way in which acquisition time depends on ω_h, I_h, and $dB_x/d\theta$. The dependence on I_h and $dB_x/d\theta$ is simple: acquisition time is proportional to I_h and inversely proportional to $(dB_x/d\theta)^2$.

The dependence of acquisition time on frequency is entirely contained in the function

$$f\left(\omega_h\right) = \frac{P^2}{\omega_h\left(A_{\text{det}} + \frac{1}{2} + n_{\text{th}}\right)}.$$

The choice $A_{\text{det}} = 16$, which is explained in the discussion preceding (4.45), along with $T_h = 10$ mK, causes $f\left(\omega_h\right)$ to have a maximum around $\omega_h/2\pi = 450\,\text{MHz}$, but the peak is fairly flat, and the value of $f\left(\omega_h\right)$ stays within 10% of the peak value for frequencies between 300 MHz and 700 MHz. If quantum-limited detection is assumed, the peak is shifted to around 525 MHz, while $f\left(\omega_3\right)$ stays within 10% of its peak value over the range 375 MHz to 775 MHz.

8 Signal-to-noise ratio for a product of correlated measurements

Reference [13] presents a SNR analysis for CONQUEST, a scheme in which an NMR spectrum is obtained by measuring a spin correlation function. The analysis in this reference does not include thermal noise in the mechanical resonator or noise added to the measurement during detection of the mechanical motion. In order to compare quantitatively the sensitivity of different techniques for NMR spectroscopy of nanoscale samples, we extend the sensitivity analysis of CONQUEST to include these forms of noise.

8.1 Definition of the signal and the noise

Since we are specifically interested in measurements which could be done with a nanoscale torsional mechanical resonator coupled to the transverse sample dipole, it will be convenient to modify the convention established in reference [13] by considering I_x rather than I_z to be the spin component measured in the CONQUEST experiment. In particular, we consider that a single shot of the experiment yields a measurement of the Heisenberg operator

$$S_2(t_1,0) = I_x(t_1)\, I_x(0) \tag{4.68}$$

$$\equiv \left(U_0^\dagger I_x U_0\right) I_x, \tag{4.69}$$

where U_0 is the spin-system evolution operator for the time period beginning at time $t = 0$ and ending at $t = t_1$. In order to simplify the discussion, we follow reference [13] in assuming that U_0 corresponds to free precession of the sample dipole at frequency ω, so that

$$\begin{aligned} I_x(t_1) &= U_0^\dagger I_x(0)\, U_0 \\ &= I_x(0)\cos\omega t - I_y(0)\sin\omega t \\ &= I_x\cos\omega t_1 - I_y\sin\omega t_1. \end{aligned} \tag{4.70}$$

Spin noise is analyzed in reference [13] by considering that each measurement is represented by a projection operator which acts on the spin system. In order to quantify the effects of instrument noise on the measurements, we replace this model with one in which a period of spin motion governed by the evolution operator U is sandwiched between two periods of spin-resonator evolution. The resonator is continuously observed throughout the experiment, with $\theta_{\mathrm{obs}}(t)$ denoting the observed value of the resonator coordinate.

In proposing a method for quantifying the information available in $\theta_{\mathrm{obs}}(t)$, we are guided by consideration of the method defined in sections 4.1 and 4.2 for analyzing the SNR of an amplitude measurement. The noisy signal $f(t)$ was defined as the torque which would produce expected displacement $\theta_{\mathrm{obs}}(t)$ in the resonator, for all t, while the "noiseless signal" $m(t)$ was defined as the torque which would produce expected displacement $\langle\theta(t)\rangle$ in the resonator, where the average is quantum statistical. The information to be extracted by analysis of $f(t)$ was the amplitude of $m(t)$, or equivalently, the value $m(0)$ at the beginning of the detection period. In order to filter out instrument noise, we multiplied $f(t)$ by $m_0(t)$ and integrated, where $m_0(t)$

has the same functional form as $m(t)$ but unit amplitude.

For CONQUEST, we propose an analogous method of analyzing SNR. Given $\theta_{\rm obs}(t)$, we find the torque $g(t)$ which would produce expected displacement $\theta_{\rm obs}(t)$ in the resonator. Our definition of the signal can be motivated by considering equation (4.39), the quantum Langevin equation for a damped resonator interacting with a spin sample:

$$\begin{aligned} I_h \frac{d^2}{dt^2}\theta(t) + \frac{2I_h}{\tau_h}\frac{d}{dt}\theta(t) + k\theta(t) &= \gamma\hbar\frac{dB_x}{d\theta} I_x(t) + N'(t) \\ &\equiv T(t) + N'(t)\,. \end{aligned}$$

The operator $N'(t)$ is a rapidly fluctuating torque of mean zero, and $T(t)$ can be identified with the torque exerted by the spins at time t. The noisy torque $g(t)$ includes contributions from $T(t)$ and $N'(t)$, as well as from noise added during the detection of the resonator's mechanical motion. Define $N_{\rm inst}(t)$ to be the torque associated with instrument noise, including both thermal noise and noise in the motion detector, and assume that the spectral density of $N_{\rm inst}(t)$ is given by (4.42). We wish to obtain from $g(t)$ a measurement of

$$\langle I_x(t_1)\, I_x(0)\rangle = \left(\frac{1}{\gamma\hbar\, dB_x/d\theta}\right)^2 \langle T(t_1)\, T(0)\rangle\,. \tag{4.71}$$

If the noiseless signal is defined by

$$m(t', t'') = \langle T(t')\, T(t'')\rangle\,,$$

and the noisy signal by

$$f(t', t'') = g(t')\, g(t'')\,,$$

then the optimal measurement protocol for CONQUEST will be the one which minimizes the variance in the estimate of

$$m(t_1, 0) = \langle T(t_1)\, T(0)\rangle \tag{4.72}$$

obtained by filtering $f(t', t'')$. Error will be introduced in the measurement due to the presence of the noise:

$$n(t', t'') = f(t', t'') - m(t', t'').$$

8.2 SNR formula

By analogy with the method of data analysis derived in section 1, we seek to express the signal $m(t', t'')$ in the form

$$m(t', t'') = G_1 m_0(t', t''),$$

where $m_0(t', t'')$ is a known function and G_1 is the value we wish to estimate. The estimate of G_1 will be given by the random variable

$$X = \frac{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(t', t'')\, m_0(t', t'')\ dt'\, dt''}{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} m_0^2(t', t'')\ dt'\, dt''}.$$

In determining the functional form of $m(t', t'')$, we neglect spin relaxation and fluctuations occurring during the interval $0 \leq t \leq t_1$. It follows from (4.70), (4.71), and (4.72) that

$$m(t_1, 0) = \left(\gamma\hbar\frac{dB_x}{d\theta}\right)^2 \left\{\left\langle I_x^2(0)\right\rangle \cos\omega t_1 - \left\langle I_x(0)\, I_y(0)\right\rangle \sin\omega t_1\right\} \tag{4.73}$$

$$= \left(\gamma\hbar\frac{dB_x}{d\theta}\right)^2 \left\langle I_x^2(0)\right\rangle \cos\omega t_1, \tag{4.74}$$

where we have assumed in moving from (4.73) to (4.74) that at time $t = 0$, the spin density matrix ρ_s is a multiple of the identity.

For simplicity, we assume that the spins exert negligible torque on the resonator during the interval $0 < t < t_1$, and so $m(t', t'') = 0$ if either t' or t'' lies in this interval. If t' and t'' lie outside this interval, then $m(t', t'')$ is proportional to the correlation function

$$C_I(t', t'') = \left\langle I_x(t')\, I_x(t'')\right\rangle.$$

In obtaining an estimate of C_I, we let let $U(t', t'')$ denote the lab-frame evolution operator for the spins, with $U(t_1, 0) = U_0$, the operator appearing in (4.69). Since we have taken $\rho_s(0)$ to be a multiple of the identity, $\rho_s(0)$ commutes with all spin operators, and C_I can be written as

$$\begin{aligned} C_I(t', t'') &= \mathrm{Tr}\{I_x(t') I_x(t'') \rho_s(0)\} \\ &= \mathrm{Tr}\{U(0, t') I_x U(t', 0) U(0, t'') I_x U(t'', 0) \rho_s(0)\} \\ &= \mathrm{Tr}\{U(t'', t') I_x U(t', t'') I_x \rho_s(0)\}. \end{aligned} \tag{4.75}$$

Equation (4.75) implies that C_I can be evaluated as the correlation function of a spin system which is completely disordered at time t''.

If t', t'' are both less than 0 or both greater than t_1, then U is the evolution operator for the spins as they drive the resonator. For simplicity, we assume that the spins are spin-locked during this period. A simple method of approximating C_I for these values of t', t'' is to assume that $\tilde{C}_I$, the correlation function in the rotating frame, is given by

$$\tilde{C}_I(t', t'') = \langle I_x^2 \rangle \exp(-|t' - t''| / T_{1\rho}),$$

where $T_{1\rho}$ is the decay time of I_x during spin-locking. We can then approximate the lab-frame correlation function as

$$C_I(t', t'') = \langle I_x^2 \rangle \exp(-|t' - t''| / T_{1\rho}) \cos(\omega_h t') \cos(\omega_h t''), \tag{4.76}$$

for $t', t'' < 0$, and

$$\langle I_x(t') I_x(t'') \rangle = \langle I_x^2 \rangle \exp(-|t' - t''| / T_{1\rho}) \cos(\omega_h(t' - t_1)) \cos(\omega_h(t'' - t_1)) \tag{4.77}$$

if $t', t'' > t_1$. Note that we have assumed that during spin-locking, components of sample dipole which are not spin-locked decay so quickly that we can neglect their contribution to the lab-frame correlation function.

If $t'' < 0$ and $t' > t_1$, we obtain

$$\begin{aligned}\langle I_x(t') I_x(t'')\rangle &= \langle U(t'',t') I_x U(t',t'') I_x\rangle \\ &= \left\langle U(t'',0) U_0^\dagger U(t_1,t') I_x U(t',t_1) U_0 U(0,t'') I_x \right\rangle,\end{aligned}$$

with the average taken for a density matrix which is a multiple of the identity. Again, this is a lab-frame correlation function, and the simplest way to approximate it is to consider first the correlation function $\tilde{C}_I$ in a particular rotating frame. For times during which the spin-locking field is present, the x-axis of this rotating frame is parallel to the resonant rotating component of the spin-locking field, while the z-axes of the rotating and lab frames are identical. During the period $0 \le t \le t_1$, the axes of the rotating and lab frames are identical (that is, the rotating frame does not rotate). In this rotating frame, we can approximate the correlation function by

$$\tilde{C}_I(t',t'') = \left\langle I_x^2 \right\rangle \cos(\omega t_1) \exp\left\{-\left(|t'-t''| - t_1\right)/T_{1\rho}\right\}. \tag{4.78}$$

Roughly speaking, equation (4.78) expresses the idea that in comparing I_x at times t'' and t' within the rotating frame, we average over a set of hypothetical, idealized measurements, and for each measurement, the following sequence of events occurs: 1) I_x is sampled at time t'', 2) Fluctuations in I_x occur during the spin-locking which lasts from $t = t''$ to $t = 0$, 3) A rotation of the spin system is performed which replaces $I_x(0)$ with $I_x(0)\cos\omega t_1 - I_y(0)\sin\omega t_1$ as the spin component along the x-axis, 4) Fluctuations in this spin component occur during the spin-locking which lasts from t_1 to t', and 5) I_x is once again sampled. Our unpolarized system has $\langle I_x I_y\rangle = 0$, and so the transverse dipole $-I_y(0)\sin\omega t_1$ directed along the x-axis at time t_1 makes no contribution to the average of these hypothetical measurements, while the effect of the fluctuations occurring during a period of length $(|t'-t''| - t_1)$ is exponential decay with time constant $T_{1\rho}$. To obtain the lab-frame correlation functions from (4.78), we once again assume that components of the sample dipole which are not spin-locked may be neglected, and we write

$$C_I\left(t',t''\right) = \left\langle I_x^2\right\rangle \cos\left(\omega t_1\right) \exp\left\{-\left(\left|t'-t''\right|-t_1\right)/T_{1\rho}\right\} \cos\left(\omega_h\left(t'-t_1\right)\right) \cos\left(\omega_h t''\right). \tag{4.79}$$

Note that when $t' < 0$ and $t'' > t_1$, we similarly obtain

$$C_I\left(t',t''\right) = \left\langle I_x^2\right\rangle \cos\left(\omega t_1\right) \exp\left\{-\left(\left|t'-t''\right|-t_1\right)/T_{1\rho}\right\} \cos\left(\omega_h t'\right) \cos\left(\omega_h\left(t''-t_1\right)\right). \tag{4.80}$$

Examination of (4.76), (4.77), (4.79), and (4.80) shows that only in the case where t' and t'' lie on opposite sides of the time interval $0 < t < t_1$ does our approximate expression for $m\left(t',t''\right)$ contain information about the precession frequency ω of the spins. In searching for an optimal method of estimating $m\left(t_1,0\right)$, we may therefore simplify the analysis by considering m to be zero in regions where t', t'' are both less than 0 or both greater than t_1. Making the assumption that $t_1 \ll T_{1\rho}$, we drop t_1 from the exponential factor appearing in (4.79) and (4.80), and we further simplify notation by redefining $m\left(t',t''\right)$ as

$$m\left(t',t''\right) = \begin{cases} \left\langle T\left(t'\right) T\left(t''+t_1\right)\right\rangle & \left(t',t''\right) \text{ in quadrant II} \\ \left\langle T\left(t'+t_1\right) T\left(t''\right)\right\rangle & \left(t',t''\right) \text{ in quadrant IV} \\ 0 & \text{otherwise} \end{cases}$$

That is, at points where the correlation function contains spectroscopic information, we define m as if the time period governed by the evolution operator U had length zero, which is a natural choice of notation within a model which neglects spin fluctuations during this time period. Our approximate expression for $m\left(t',t''\right)$ then becomes

$$m\left(t',t''\right) = \left(\gamma\hbar\frac{dB_x}{d\theta}\right)^2 \left\langle I_x^2\right\rangle \cos\left(\omega t_1\right) \exp\left(-\left|t'-t''\right|/T_{1\rho}\right) \cos\left(\omega_h t'\right) \cos\left(\omega_h t''\right)$$

at all points $\left(t',t''\right)$ lying in quadrant II or quadrant IV of the plane. The estimate

$f(t', t'')$ of the useful signal is also redefined so that

$$f(t', t'') = m(t', t'') + n(t', t'') \tag{4.81}$$

for all points (t', t'') in the plane, including points at which $m(t', t'') = 0$.

The information which we wish to extract from a single shot of a CONQUEST experiment is an estimate of

$$G_1 \equiv \left(\gamma\hbar \frac{dB_x}{d\theta}\right)^2 \langle I_x^2 \rangle \cos(\omega t_1). \tag{4.82}$$

Our simplified notation for $m(t', t'')$ allows us to define $m_0(t', t'')$ by the equation

$$m(t', t'') = G_1 m_0(t', t'').$$

The analysis used to find the optimal linear filter for transverse BOOMERANG can be carried over without substantial modification to show that the optimal estimate of G_1 is given by

$$X = \frac{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(t', t'')\, m_0(t', t'')\; dt'\, dt''}{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} m_0^2(t', t'')\; dt'\, dt''} \tag{4.83}$$

if the noise is white.

The noise in the function $f(t', t'') = g(t')\, g(t'')$ will include contributions from the products $T(t')\, T(t'')$ of spin torques, the products $N_{\text{inst}}(t')\, N_{\text{inst}}(t'')$ of torques associated with instrument noise, and the products $T(t')\, N_{\text{inst}}(t'')$ and $N_{\text{inst}}(t'')\, T(t')$ of one spin torque and one torque associated with instrument noise. We shall assume that the dominant noise source contributing to $g(t')\, g(t'')$ comes from the product $N_{\text{inst}}(t')\, N_{\text{inst}}(t'')$. This would occur for a problem in which

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} T(t')\, T(t'')\, m_0(t', t'')\; dt'\, dt''$$

and

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} T(t')\, N_{\text{inst}}(t'')\, m_0(t', t'')\; dt'\, dt''$$

are substantially smaller than

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} N_{\text{inst}}(t')\, N_{\text{inst}}(t'')\, m_0(t',t'')\; dt'\, dt'',$$

that is, a problem in which the products $T(t')\,T(t'')$ and $T(t')\,N_{\text{inst}}(t'')$ have much smaller components in the relevant frequency domain than $N_{\text{inst}}(t')\,N_{\text{inst}}(t'')$. An example of such a problem would be the two-spin system of section 1.2 of chapter 6, with the spectrum detected by the example resonator of table 5.3 and the noise temperature $T_N = 18T_{QL}$. A more general SNR expression could be obtained by estimating the spectral densities of the noise contributions due to the products $T(t')\,T(t'')$ and $T(t')\,N_{\text{inst}}(t'')$.

The instrument noise characterized by equation (4.42) is flat within the spectral range of interest, and so the instrument noise at distinct sampled times $t' \neq t''$ can be considered independent. The unfiltered noise $n(t',t'')$ can therefore be approximated as the product of two normally distributed random variables, denoted by $n_{\text{inst}}(t')$ and $n_{\text{inst}}(t'')$:

$$n(t',t'') = n_{\text{inst}}(t')\, n_{\text{inst}}(t'')\,.$$

The correlation function C_n of the noise is defined as

$$\begin{aligned} C_n(t'_1,t''_1,t'_2,t''_2) &= \langle n(t'_1,t''_1)\, n(t'_2,t''_2)\rangle \\ &= \langle n_{\text{inst}}(t'_1)\, n_{\text{inst}}(t''_1)\, n_{\text{inst}}(t'_2)\, n_{\text{inst}}(t''_2)\rangle\,. \end{aligned}$$

Note that the four random variables $n_{\text{inst}}\left(t'_j\right)$, $n_{\text{inst}}\left(t''_j\right)$ may be considered independent, since we are not concerned with the small subset of sampled points at which two or more of the times are identical. We thus have

$$\begin{aligned} C_n(t'_1,t''_1,t'_2,t''_2) &= \langle n_{\text{inst}}(t'_1)\, n_{\text{inst}}(t'_2)\rangle\, \langle n_{\text{inst}}(t''_1)\, n_{\text{inst}}(t''_2)\rangle \\ &= C_{\text{inst}}(t'_2 - t'_1)\, C_{\text{inst}}(t''_2 - t''_1)\,, \end{aligned}$$

where $C_{\text{inst}}(t)$ is the correlation function of the instrument noise $n_{\text{inst}}(t)$. We can thus write C_n as a function of two variables:

$$C_n(t', t'') = C_{\text{inst}}(t')\, C_{\text{inst}}(t'').$$

The double-sided spectral density $S_n(\omega', \omega'')$ of n is

$$S_n(\omega', \omega'') = S_{\text{inst}}(\omega')\, S_{\text{inst}}(\omega''),$$

where $S_{\text{inst}}(\omega)$ is given by equation (4.42).

The variance introduced into the estimate X by instrument noise is

$$\sigma^2_{\text{inst}} = \frac{\left(S_{\text{inst}}(\omega_h)\right)^2}{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} m_0^2(t', t'')\; dt'\, dt''}. \tag{4.84}$$

Note that noise at points (t', t'') lying in the first and third quadrants makes no contribution to the estimate X, since m_0 is zero in these regions. Since

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} m_0^2(t', t'')\; dt'\, dt'' \approx \frac{T_{1\rho}^2}{16},$$

we have

$$\sigma^2_{\text{inst}} = \left(\frac{4S_{\text{inst}}(\omega_h)}{T_{1\rho}}\right)^2. \tag{4.85}$$

It follows from equations (4.82) and (4.85) that the SNR is

$$\begin{aligned} SNR_{\text{CONQUEST}} &= \frac{\left(\gamma\hbar\, dB_x/d\theta\right)^2 \langle I_x^2\rangle \cos(\omega t_1)}{\left(4S_{\text{inst}}(\omega_h)/T_{1\rho}\right)} \\ &= N\left(\frac{\gamma\hbar}{2}\frac{dB_x}{d\theta}\right)^2 \frac{1}{4S_{\text{inst}}/T_{1\rho}}. \end{aligned} \tag{4.86}$$

8.3 Comparison of the first-order and second-order methods

In comparing the sensitivity of the "first-order" method which measures a single value of $\langle I_x(t_1)\rangle$ and the "second-order" method which measures $\langle I_x(t_1)\, I_x(0)\rangle$, we consider detection at a single point t_1 for which $\cos(\omega t_1) = 1$. If spin-locking is used to detect

$\langle I_x(t_1)\rangle$, the results of section 4.5 imply that the single-shot SNR is

$$SNR_{\mathrm{BOOM}} = PN\frac{\gamma\hbar}{2}\frac{dB_x}{d\theta}\sqrt{\frac{1}{4S_{\mathrm{inst}}/T_{1\rho}}}, \tag{4.87}$$

where the subscript "BOOM" highlights the fact that this method of measuring an NMR spectrum is a version of the BOOMERANG scheme for force-detected spectroscopy in the absence of field gradients [13]. Comparison of (4.86) and (4.87) shows that for a sample consisting of a single spin with polarization $P = 1$, we have

$$SNR_{\mathrm{CONQUEST}} = \left(SNR_{\mathrm{BOOM}}\right)^2.$$

In this case, the contribution of instrument noise to the measurement of $\langle I_x(t_1)\, I_x(0)\rangle$ equals the product of the instrument noise for independent measurements of $\langle I_x(t_1)\rangle$ and $\langle I_x(0)\rangle$.

More generally, we have

$$\begin{aligned} SNR_{\mathrm{CONQUEST}} &= \frac{1}{P^2 N}\left(SNR_{\mathrm{BOOM}}\right)^2 \\ &= \left(\frac{SNR_{\mathrm{BOOM}}}{P^2 N}\right) SNR_{\mathrm{BOOM}} \end{aligned} \tag{4.88}$$

if instrument noise is dominant. Equation (4.88) may be considered a generalization of the result that when spin noise is dominant [13],

$$\begin{aligned} SNR_{\mathrm{BOOM}} &= P\sqrt{N}, \\ SNR_{\mathrm{CONQUEST}} &= \frac{1}{\sqrt{1 + (1 - 2/N)}} \\ &\approx 1, \end{aligned}$$

since (4.88) holds in this case as well. When (4.88) holds, e.g., when either the spin noise or instrument noise can be neglected, the second-order method is more sensitive than the first-order method provided that

$$SNR_{\mathrm{BOOM}} \geq P^2 N. \tag{4.89}$$

When instrument noise is dominant, (4.89) can be expressed as

$$\frac{\gamma\hbar}{2}\frac{dB_x}{d\theta}\sqrt{\frac{1}{4S_{\mathrm{inst}}/T_{1\rho}}} \geq P. \tag{4.90}$$

Equation (4.90) implies that the second-order method is preferred if the sample polarization P is less than the single-shot SNR for detecting a single spin which is aligned along the x-axis at the beginning of the detection period.