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Phys. Rev. A **84**, 052315 — Published 15 November 2011

DOI: [10.1103/PhysRevA.84.052315](https://doi.org/10.1103/PhysRevA.84.052315)

Characterization of a qubit Hamiltonian using adaptive measurements in a fixed basis

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We investigate schemes for Hamiltonian parameter estimation of a two-level system using repeated measurements in a fixed basis. The simplest (Fourier based) schemes yield an estimate with a mean square error (MSE) that decreases at best as a power law $\sim N^{-2}$ in the number of measurements N . By contrast, we present numerical simulations indicating that an adaptive Bayesian algorithm, where the time between measurements can be adjusted based on prior measurement results, yields a MSE which appears to scale close to $\exp(-0.3N)$. That is, measurements in a single fixed basis are sufficient to achieve exponential scaling in N .

PACS numbers: 03.67.-a, 03.65.Wj

I. INTRODUCTION

Efficient methods for the characterization of quantum systems to extremely high precision are important both to reach new regimes of physics and to build robust quantum technologies [1, 2]. One of the most fundamental characterisation tasks is the estimation of the parameters of a Hamiltonian in a two-level system. Several previous studies [3–5] used a method of repeatedly initializing the two-level system and then performing measurements in a fixed basis after consecutively longer intervals (during which the system evolves under its Hamiltonian) and then averaging many runs. By calculating the Fourier transform of the resulting signal and identifying its peak, it is possible to obtain an estimate for the rate of evolution, and thus the desired Hamiltonian parameter.

This approach is noticeably more efficient (faster) in practice than quantum process tomography [6], requiring only measurements in one particular basis (as state initialization can be done via measurement). However, it still demands a large number of measurements for moderate accuracy. For example, in Ref. [3], the two parameter estimation procedure required at least 10^6 measurements in order to reach a joint variance of 10^{-3} in the parameters being estimated. Such large numbers of measurements can pose a problem, especially in solid-state systems where the measurement time is typically the slowest timescale, often many orders of magnitude longer than the period for coherent evolution. To specifically address such situations, we quantify resources in our estimation schemes as N , the number of measurements used, rather than the total evolution time as is commonly used in phase estimation schemes using optics and assuming instantaneous measurements [7] (however cf. [8]). We note however that our techniques could easily be modified to take into account both the waiting time

and the measurement time.

We emphasise that, unlike schemes based on the quantum phase estimation algorithm [1, 10] such as that proposed in Refs. [8, 9], we restrict our measurement to a fixed basis and do not allow any controlling unitary dynamics. That is, our schemes are limited to preparing a pure state in this fixed basis, evolving for some time under the Hamiltonian, and measuring in this same basis. The motivation for this restriction is simple: in most situations, the unitary required to change bases would be generated by the very Hamiltonian parameter that we are attempting to estimate.

A motivating example is provided by recent experimental progress in the development of spin qubits in semiconductor quantum dots, specifically, GaAs double dot systems where a qubit is defined using two electron spins in a singlet/triplet configuration [11]. With one electron in each dot, the states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ experience an energy splitting proportional to the difference in the z -component of the magnetic field, ΔB^z , resulting from the hyperfine interaction with nearby lattice nuclear spins. Because variations in ΔB^z are the primary source of decoherence in these spin qubits, there has been considerable recent interest in the measurement and control of this nuclear magnetic field by using the spin qubit as both a probe and feedback mechanism [12–15]. In addition, a well-known and stable value of this field can serve as a source of coherent quantum operations (i.e., logic gates) on the spin qubit [14, 15]. (However, one cannot use this effect to change the measurement basis and implement a quantum phase estimation algorithm as in [1, 8, 10] without first estimating the field; thus, our requirement for fixed basis measurements.) With the recent demonstration of single-shot projective measurements of the spin qubit [16], parameter estimation of ΔB^z in such systems is possible [15]. The system coherently evolves on a nanosecond timescale, whereas the measurement time is $\sim 10\mu\text{s}$ [14, 17, 18]. (In these systems the coherent evolution is switched off during the measurement process.) For this estimation problem, then, we seek schemes that min-

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imize the number of measurements required for a given accuracy.

In this paper, we consider the performance of a range of schemes for such a parameter estimation, using numerical simulations. First, we demonstrate that a Bayesian approach outperforms the Fourier estimation techniques. We show that, while schemes using a predetermined sequence of measurements yield a mean square error (MSE) decreasing polynomially in the number of measurements, a drastic improvement can be found by using *adaptive* measurement approach [2]. The adaption is done by *local optimization* [19]: the time intervals between preparation and measurement is chosen to minimize the expected MSE, conditioned on the result of that future measurement. Numerical simulations for the adaptive scheme are consistent with exponential scaling in N for the MSE in the estimate of the parameter, while the best nonadaptive algorithm found has a power law scaling in N . Our result demonstrates that exponential scaling of the estimate precision can be achieved with a single, fixed basis of measurement, rather than requiring measurements in arbitrary bases as in the quantum phase estimation algorithm [1, 8, 10]. Finally, we show that quite good performance is achievable by a *locally optimal non-adaptive* scheme.

II. THE PROBLEM

We consider the problem of estimating a single unknown parameter of a qubit Hamiltonian, of the form $H = \omega\sigma_z/2$. To simplify later calculations we assume that ω is a random parameter uniformly distributed over the interval $[0, \omega_0]$, where ω_0 is the largest possible value of ω . In order to estimate ω , we probe that system with projective measurements of the x component of spin at different times. (Note that this measurement basis is *not* the energy eigenbasis of the Hamiltonian; otherwise, parameter estimation would not be possible.) We initialize the state as an eigenstate $|+\rangle$ of σ_x at $t = 0$; we note that this initialization is naturally performed at each step by the previous measurement. The Nyquist–Shannon theorem suggests that we want to choose the time between preparation and measurement to be as small as $\tau \equiv \pi/\omega_0$. This minimum time interval τ (and hence maximum parameter range $[0, \omega_0]$) will be determined by experimental considerations, and it is therefore reasonable to assume that the *waiting time* between the k th preparation and the k th measurement, is an integer multiple of τ . That is, $t_k = m_k\tau$. The Hamiltonian in this case generates the time evolution

$$|\psi(t)\rangle = \cos(\omega t/2)|+\rangle - i \sin(\omega t/2)|-\rangle, \quad (1)$$

and the probabilities for the outcomes of the k th measurement are

$$p_k(+|\omega) = \cos^2\left(\frac{\pi\omega m_k}{2\omega_0}\right), \quad p_k(-|\omega) = \sin^2\left(\frac{\pi\omega m_k}{2\omega_0}\right). \quad (2)$$

The relevant resource in our estimation procedure is the number of measurements. The problem then becomes: given a fixed number of measurements N , how should one proceed in determining the waiting times $m_k\tau$, and how does one infer ω from the results of the measurements?

This problem falls within the domain of *quantum parameter estimation*, wherein one seeks to identify an unknown parameter influencing the preparation or dynamics of a quantum system. The canonical example is estimating the phase of a unitary operator, which is closely related to characterizing a Hamiltonian with an unknown magnitude, as in this paper. Quantum parameter estimation techniques can allow for high-precision phase estimation below the classical (shot noise limit) as well as power algorithms for quantum computation [1, 10]. In quantum parameter estimation problems, such as the one we consider, it is necessary to carefully tailor measurements and process their outcomes in order to make inferences on the (unaccessible) parameter of interest. While many techniques for quantum parameter estimation make use of entanglement [20], it is in some situations possible to replace entangled states with repeated application of the unknown unitary on a single system prior to measurement [7, 21, 22]. Adaptive measurements—which have been proposed and used for quantum parameter estimation [7–9, 19, 23–25], quantum tracking [26, 27], state discrimination [28, 29], state estimation [30–32], and quantum computing [33–35]—can play a key role in this context because of the phase ambiguity inherent in estimating a parameter that appears in the problem only as the scale of an anti-Hermitian operator (i.e. $-iHt$) which is exponentiated [7, 22].

One question of interest in quantum parameter estimation is how close the measurement comes to the so-called Heisenberg limit [2]. This is the limit on the variance, or Fisher information, of the unknown parameter, imposed by Heisenberg’s uncertainty principle. For example, in the case of phase estimation, this limit scales as N_U^{-2} , where N_U is the total number of times the unitary is applied, whether it is applied N_U times to a single system, or once each across N_U systems, or anything in between [20, 22]. Restricting to a single system (as in our paper), in the asymptotic limit $N_U \rightarrow \infty$, the run-time of any experiment that can attain the Heisenberg limit will scale as N_U . However, as noted above, in the practical regime of interest to us, the run-time of the experiment will be determined by N , the number of preparation and measurement steps, not the evolution time $\sim N_U$ between preparation and measurement. Since there is no fixed relation between N_U and N (except that $N_U \geq N$), the Heisenberg limit does not automatically translate into any limit on the variance as a function of N . Rather, we must determine how well various schemes scale with N (in the regime of interest), and thereby determine the best of them.

III. SCHEMES FOR PARAMETER ESTIMATION

In the following sections, we present techniques for Hamiltonian parameter estimation based on Fourier methods (A), and then those based on Bayesian methods (B–D). The latter include simple non-adaptive Bayesian schemes (B), our locally optimal adaptive Bayesian scheme (C), and a locally-optimal non-adaptive Bayesian scheme (D).

A. Fourier Estimation Techniques

A simple strategy for this problem is to measure at uniformly distributed times $t_k = k\tau$, i.e., to choose $m_k = k$. The set of measurement results constitutes a measurement record, and can be loosely thought of as one realization of a random process [5]. One method to estimate the parameter is to Fourier transform the measurement record and identify the peak of the spectrum as the best estimate for ω [3, 4]. However, this is not the only strategy. For example, for each $t = m\tau$ we could prepare, evolve and measure twice, with the range $m \in \{1, \dots, N/2\}$. The resulting measurement record can be viewed as two realizations of the random process, and averaging these two realizations will reduce the effect of projection noise (i.e., the noise due to the indeterminacy of the measurement outcomes). We can define a family of schemes, wherein M different choices of waiting times are each repeated n times, with a total of $N = nM$ measurements.

Using this technique we have considered partitions of N where $n \in \{1, 2, 3, \dots, 10\}$. We find that $n \in \{1, 2, 3\}$ give the best MSE scaling depending on the value of N ; see Fig. 1. In what follows, we use the partitioning that minimizes the MSE for a given N , and call this method the *best Fourier method*. The MSE in the estimate of ω as a function of N for this method sets the benchmark to which our more sophisticated schemes will be compared. For a large number of measurements N , the scaling of the MSE is found to have power-law scaling in N with a power close to -2 . Specifically, for a fit of N from 36 to 3000 with each point sampled 400 times, the 95% confidence interval in the power is $(-2.096, -2.064)$, $R^2 = 0.956$.

B. Bayesian Parameter Estimation

We now consider performing a Bayesian analysis of the same schemes described above. Here, one's knowledge about the unknown parameter ω is represented as a probability distribution $P(\omega)$. Using the mean of this distribution as one's estimate gives a MSE which is equal to the variance of this probability distribution, averaged over all realizations. Thus we can use the variance of the

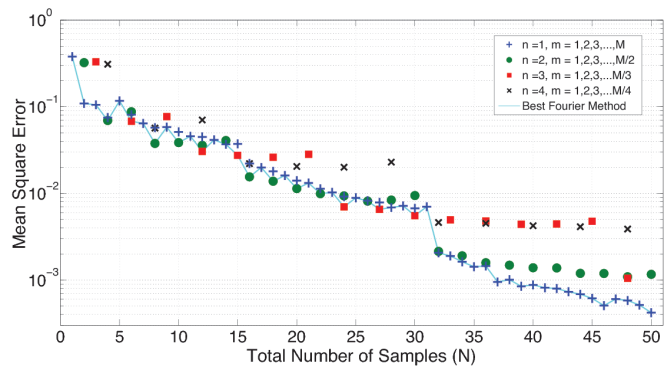


FIG. 1: The MSE in the frequency estimate for Fourier-based schemes for some different partitionings of N . The “Best Fourier Method” (solid line) for a particular N is given by the best performing scheme for that N . To generate the data for this plot each scheme was sampled 100 000 times, consequently the error bars (not shown) are slightly smaller than the markers for the data points.

posterior (i.e. post-measurement) $P(\omega)$ as the measure of precision for Bayesian schemes.

We take the uniform prior probability distribution $P_0(\omega) = 1/\omega_0$. At each measurement, the outcomes $+$ and $-$ are expected with probabilities given by Eq. (2) and so the total probability distribution can be updated each measurement step using Bayes rule. The general expression for conditioned probability distribution of ω given k measurements, is

$$P_k(\omega|r_k \dots r_1) = \mathcal{N} \prod_{j=1}^k [1 + r_j \cos(\pi m_j \omega / \omega_0)], \quad (3)$$

where $r_j = 1$ ($r_j = -1$) corresponds to learning that the j th result is $+$ ($-$), m_j denotes the waiting time for the k th measurement, and \mathcal{N} is a normalization constant. These conditional probabilities allow for any Bayesian parameter estimation task to be performed on a given measurement record.

We can avoid the computationally costly practice of discretizing the distribution in ω by using the following technique. As Eq. (3) is an even function of ω , it can be represented as a Fourier cosine series:

$$P_k(\omega|r_k \dots r_1) = \frac{1}{2} c_k(0) + \sum_{q=1}^N c_k(q) \cos(q\pi\omega/\omega_0), \quad (4)$$

where $N = \sum_{j=1}^k m_j$. The distribution is normalized by dividing by $\frac{1}{2}\omega_0 c_k(0)$. Because the number of terms in Eq. (4) is finite, the representation of the distribution is exact. It is then possible to derive an analytic expression for $\langle \omega \rangle = \int_0^{\omega_0} \omega P_k(\omega|r_k \dots r_1) d\omega$ (and $\langle \omega^2 \rangle$) using the Plancherel theorem, which relates the convolution of two functions, $P_k(\omega|r_k \dots r_1)$ and ω (or ω^2), to the summation of the product of their corresponding Fourier coefficients. Performing this calculation gives an explicit

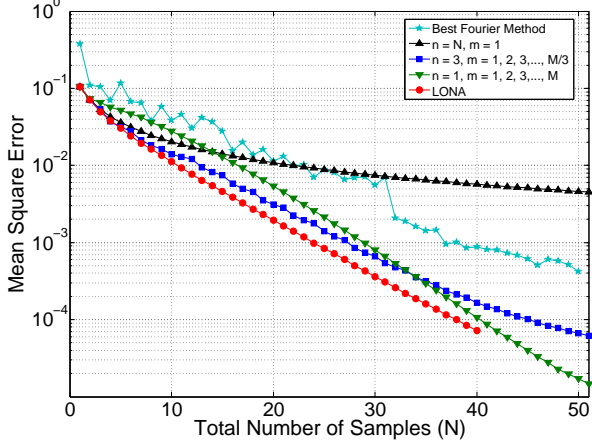


FIG. 2: A comparison of the scaling of the variance for Fourier and non-adaptive Bayesian methods. The stars are for the Best Fourier method described in the text. The upward triangles are for the Bayesian method where the N samples are taken at $m = 1$. The downward triangles are for the Bayesian $n = 1$ method where the N samples are sequentially taken at times $m = 1, 2, 3, \dots, M$ (here $M = N$). The squares are for the Bayesian $n = 3$ method where each point is sampled three times, i.e., $m = 1, 1, 1, 2, 2, 2, \dots, M/3$. The circles are for the locally optimal non-adaptive (LONA) method.

formula for the variance, $V = \langle \omega^2 \rangle - \langle \omega \rangle^2$, given by

$$V = \left[\frac{\omega_0^2}{3} + \sum_{q=1}^N \frac{2c_q \omega_0^2 (-1)^q}{c_0 (q\pi)^2} \right] - \left[\frac{\omega_0}{2} + \sum_{q=1}^N \frac{c_q \omega_0 [(-1)^q - 1]}{c_0 (q\pi)^2} \right]^2. \quad (5)$$

With this technique, we can perform a Bayesian analysis of the measurement outcomes of the predefined parameter estimation schemes discussed above. We simulated over 100 000 runs for $n \in \{1, 2, 3\}$ and N up to 36 measurements to obtain the variance as a function of N shown on Fig. 2. The simplest algorithm with $n = N$, $m = 1$ yields an asymptotic scaling of the variance $\sim N^{-1}$. This is obtained by fitting the first 5000 steps (95% confidence interval of power law scaling (0.9893, 0.9895), with $R^2 > 0.9999$). By contrast, algorithms with $n \in \{1, 2, 3\}$ that uniformly distribute measurement times exhibit an improved error scaling of the variance $\sim N^{-3}$ (for $n = 1$, the first 1000 steps yield the 95% confidence interval for the power to be (3.0376, 3.0384), with $R^2 > 0.9999$). This latter result demonstrated a significant improvement over the Fourier analysis using the same sequences, an improvement due solely to the superior data processing of Bayesian analysis. We find that $n = 3$ is the most effective for smaller N (likely due to a reduction in projection noise), whereas $n = 1$ has a better scaling for large N .

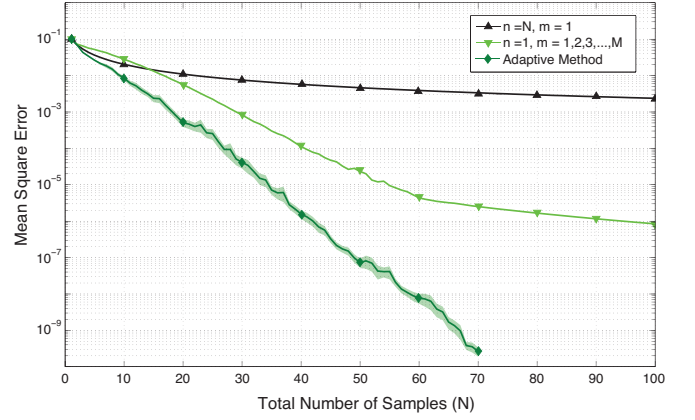


FIG. 3: The plots for mean square error as a function of the total number of measurements: (\blacktriangle) the Bayesian method where the N samples are taken at $m = 1$; (\blacktriangledown) the Bayesian method where the N samples are sequentially taken at times $m = 1, 2, 3, \dots, M$; (\blacklozenge) the locally optimal adaptive strategy. The average MSE was computed from 10 000 simulations and the largest possible allowed waiting time was $m_{max} = 1000$. The shaded region on the adaptive strategy plot represents the standard deviation of the MSE.

C. Adaptive Bayesian Scheme

We next consider an adaptive method in which the waiting times t_k are chosen based on previous results. Specifically, we adaptively chose m_k so that the conditional expectation of the variance $E[V]$ after the measurement is minimized. The conditional expectation of the variance after the k th result for the waiting time m_k is

$$E[V_k | m_k] = \frac{c_k(0|+)V_{k|+} + c_k(0|-)V_{k|-}}{c_k(0|+) + c_k(0|-)} \quad (6)$$

where $c_k(0|r)$ denotes the Fourier coefficient $c_k(0)$ of Eq. (4) given the measurement outcome r from the k th measurement and $V_{k|r}$ is the variance conditional on this outcome. The factors multiplying each V_r are the probabilities of the outcomes. Our strategy is to, at each step, choose the waiting time τm_k in order to minimize the expected variance of posterior distribution $E[V_k | m_k]$.

Fig. 3 shows the scaling of the variance as a function of N for this adaptive strategy, compared with the above non-adaptive Bayesian schemes. Unlike the previous schemes where we could fit numerics beyond $N = 200$, here we are limited up to $N = 70$. Fitting to the first 70 measurements, the MSE of this adaptive strategy scales as $\sim \exp(-aN)$ with $a = 0.2990$ (with 95% confidence interval for exponent a of (0.2796, 0.3185)) and $R^2 = 0.9847$. We compare this exponential fit with the best power fit, which gives $\sim N^{-7}$ with R^2 of only 0.9064. That is, we have obtained an exponentially decreasing MSE similar to that of Ref. [8] without the need to alter measurement bases throughout the protocol.

While scaling in the number of steps can be exponen-

Algorithm	Steps to $V = 10^{-3}$	Steps to $V = 10^{-5}$
Bayesian $n = N$	242	$\gtrsim 2 \cdot 10^4$
Fourier	33	$\gtrsim 130$
Bayesian $n = 1$	29	55
LONA	24	49
Adaptive	20	35

TABLE I: Comparison of schemes. Number of measurements required to meet a desired variance of 10^{-3} and 10^{-5} .

tial in N , this does not mean breaking the Heisenberg limit on the variance, scaling as N_U^{-2} . The reason is that the adaptive algorithm (as well as other previously discussed schemes) require exponentially longer waiting times for large number of steps, so that N_U varies exponentially with N . As noted above, in the truly asymptotic regime, the evolution time will become much longer than the measurement time. In that limit our algorithm will scale worse than the Heisenberg limit in terms of total run-time, since it is optimized for a different problem.

D. Locally Optimal Non-Adaptive Scheme

Due to the computation required in optimally choosing the waiting time at each measurement step, the complexity of the adaptive scheme could present problems for practical use. We therefore seek to identify non-adaptive schemes with the best possible performance. Several heuristics enable one to design such schemes; we will describe one.

In the initial step, we begin with a flat prior and determine what waiting time will minimize $E[V_1|m_1]$. For the second measurement, we determine the optimal waiting time to minimize $E[V_2|m_2]$ given that a measurement was performed at m_1 but the result is not known. This process is then repeated. We can find the first 20 steps analytically — i.e., $\{m_1, m_2, m_3, m_4, m_5, \dots\} = \{1, 1, 2, 1, 3, \dots\}$. After that, we use a numerical search. Because these waiting times are determined from expected rather than actual statistics, it is non-adaptive; this string of waiting times is determined offline. We denote this scheme the locally optimal non-adaptive (LONA) scheme. Because of computational complexity, it becomes intractable to determine the error scaling of LONA for large number of steps. However this algorithm performs well for small N (see Fig. 2), and so is appealing in situations where relatively few measurements are necessary and adaptive methods are not feasible.

IV. DISCUSSION

We have shown that Bayesian methods can be used for efficient Hamiltonian parameter estimation schemes.

Our adaptive Bayesian algorithm, which is locally optimal, provides an exponential improvement in the scaling of the variance with the number of measurements performed, and unlike methods based on the quantum phase estimation algorithm does not require adaptive measurement bases — the measurements are in a fixed basis and only the waiting times between them are adapted. See Table I for a comparison of schemes.

We note that decoherence will in general affect the performance of these schemes. Recently, considerable progress has been made in the understanding of how to determine asymptotic limits in parameter estimation in the presence of decoherence [36]. While a detailed analysis of the effects of decoherence is beyond the scope of this work, we note that simulations based on realistic parameters for GaAs double dot spin qubits possessing coherent evolution on the nanosecond timescale and dephasing times of microseconds demonstrate only a small effect on the performance of the LONA scheme up to ~ 30 measurements.

We emphasize that, in our analysis, we have used the number of measurements N to represent the resource cost of the scheme; this differs from typical phase estimation scenarios, where N represents the total number of applications or probes (e.g., number of photons) of the Hamiltonian [20]. As such, the scalings of our various schemes cannot be directly compared with other results, nor the terminology based around the standard quantum limit or the Heisenberg limit. For a simple comparison, it should be noted that the waiting time in our schemes typically becomes exponentially long for large N , and so even the adaptive Bayesian scheme with its exponential scaling in terms of number of measurements N will appear Heisenberg-limited when total time is used instead.

Acknowledgments

The authors would like to acknowledge fruitful conversations with Jared H. Cole, Jason F. Ralph, and David Reilly. This research was supported by the Australian Research Council Centre of Excellence scheme (project numbers CE110001027 and CE110001013). SDB acknowledges support from ARO/IARPA project W911NF-10-1-0330. JC acknowledges support from National Science Foundation Grant No. PHY-0903953 and Office of Naval Research Grant No. N00014-11-1-008.

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