**Capability comparison of quantum sensors of single or two qubits for a spin chain system**

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Abstract: Quantum sensing, utilizing quantum techniques to extract key information of a quantum (or classical) system, is a fundamental area in quantum science and technology. For quantum sensors, a basic capability is to uniquely infer unknown parameters in a system based on measurement data from the sensors. In this paper, we investigate the capability of a class of quantum sensors for a spin-$\frac{1}{2}$ chain system with unknown parameters. The sensors are composed of qubits which are coupled to the object system and can be initialized and measured. We consider the capability of the single- and two-qubit sensors and show that the capability of single-qubit quantum sensors can be enhanced by adding an extra qubit into the sensor under a certain initialization and measurement setting.

Keywords: Quantum sensing, qubit sensor, spin chain system.

1. INTRODUCTION

Quantum sensing is a newly emerging area which refers to the use of quantum apparatus to measure a physical quantity (quantum or classical) (Degen et al., 2017). With high sensitivity and precision, many elementary quantum systems, such as atomic spin systems, NV center ensembles and trapped iron, serve as good quantum sensors and are widely used to detect physical quantities such as magnetic fields, electric fields, temperature, etc. (Bonato and Berry, 2017). Potential applications of quantum sensors include: precision metrology (Giovannetti et al., 2011), quantum control (Dong and Petersen, 2010; Dong et al., 2019; Guo et al., 2019; Shu et al., 2020; Wiseman and Milburn, 2014), quantum experimental design, quantum system identification (Burgarth and Maruyama, 2009; Wang et al., 2019; Yu et al., 2019b; Gao et al., 2016), etc. Research efforts have been devoted to the design of new quantum sensors to enhance their sensibility and precision or to carry out tasks that are impossible using classical methods (Degen et al., 2017; Bonato and Berry, 2017).

This paper analyses the capabilities of a class of quantum sensors (qubit sensors), where qubit systems are employed for sensing tasks. Qubit systems are relatively easy to be controlled and measured, which makes them useful quantum sensors (Nakamura et al., 2017; Shi et al., 2013; Campbell and Hamilton, 2017; Qi et al., 2017). The object system of interest is a quantum spin-$\frac{1}{2}$ chain system whose Hamiltonian is par-tially given but with unknown parameters (Cappellaro et al., 2007; Jurcevic et al., 2014). The estimation of these unknown parameters is a significant problem and many efforts have been devoted to this area (Bonnabel et al., 2009; Burgarth et al., 2009; Burgarth and Maruyama, 2009; Wang et al., 2018; Zhang and Sarovar, 2014; Wang et al., 2018, 2019). The sensing qubits are coupled to the object system in a specified pattern. As illustrated in examples, the sensors are also chosen to be spin-$\frac{1}{2}$ systems.

In this paper, we define the capability of a sensor to be determined by whether the data obtained by the sensor can be used to estimate all of the unknown parameters in the system Hamiltonian, without ambiguity. We first consider and analyse a single-qubit sensor where only one spin is coupled to the object system and is then probed using a specified measurement scheme (Nakazato et al., 2003; Kato and Yamamoto, 2014). We show that the initial setting and the measurement should match, otherwise the sensor fails to uniquely determine all of the unknown parameters. For the initial settings where the single-qubit sensor fails, we propose to employ a two-qubit sensor and design a scheme to successfully carry out the sensing task.

The remainder of this paper proceeds as follows. In Section 2, we introduce the dynamical modeling of qubit sensors for spin chain systems. Initialization and measurement constraints are specified and the concept of sensing capability is introduced. In Section 3, we analyse the performance of single-qubit sensors and concentrate on a case in which single-qubit sensors fail to uniquely determine all of the unknown parameters. Then a two-qubit sensing scheme is proposed in Section 4 and its sensing capability is confirmed. Conclusions are presented in Section 5.
2. DYNAMICAL MODELING AND BASIC SETTINGS

2.1 Qubit sensor

Qubit systems may serve as excellent sensors for information detection (Sone and Cappellaro, 2017; Wang et al., 2018; Poggioli et al., 2018). A qubit system can be a spin-\( \frac{1}{2} \) system, a two-level atom or a particle in a double-well potential. In this paper, a number of spin-\( \frac{1}{2} \) systems are employed as the qubit sensor. The angular momentum of a spin-\( \frac{1}{2} \) system can only take values of \( \pm \frac{1}{2} \) when measured in any direction, which makes it a two-state system (Griffiths and Schroeter, 1995). Specifically, we study a class of qubit sensors where several selected qubits are coupled to the object system and their dynamics may contain information about the system. The information of interest for the object system can be acquired by probing (i.e., measuring) the sensor.

A two dimensional complex valued vector can describe the state of a spin-\( \frac{1}{2} \) system, which can be further expressed as the following linear combination

\[
|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle.
\]

Here, \( \alpha \) and \( \beta \) are complex numbers satisfying the relationship

\[
|\alpha|^2 + |\beta|^2 = 1,
\]

and \( |\uparrow\rangle \) represents the state of ‘spin up’ and \( |\downarrow\rangle \) represents the state of ‘spin down’. We may denote

\[
|\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.
\]

The following Pauli matrices

\[
\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},
\]

together with the identity matrix \( I \), form a complete bases for the observable space of a qubit system. Later on we also write \( X := \sigma_x, Y := \sigma_y \) and \( Z := \sigma_z \).

Note that Pauli operators are non-commuting which means Pauli measurements are not compatible with each other. The eigenstates of the Pauli matrices, corresponding to their eigenvalues \( \pm 1 \), are as follows

\[
|\psi_{+}\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad |\psi_{-}\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix},
\]

\[
|\psi_{\uparrow}\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix}, \quad |\psi_{\downarrow}\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix},
\]

\[
|\psi_{z}\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |\psi_{\overline{z}}\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.
\]

2.2 Qubit sensor for a spin-\( \frac{1}{2} \) chain system

Identifying the unknown coupling strengths in a spin system is one of the basic tasks to study and control a range of quantum phenomena (Jurcevic et al., 2014). The chain system is usually regarded as a gray box, which means it can not be initialized, manipulated or measured (see the right part of the box in Figure 1), even if some limited prior knowledge on the structure of the object system can be obtained. Therefore, the initial state of the object system is assumed to be in the maximally mixed state. The spins in the object chain system only interact with their adjacent spins. Hence, usually the only practical way to have access to the chain system is through a quantum sensor, which can be both initialized and measured.

To determine the sensing capability of a quantum sensor, a dynamic model of the whole system including both the sensor and the object spin chain system is required. The method employed varies according to the dynamical modeling and a good dynamic model can benefit the process of capability determination. For the single-qubit case, we employ the state space model proposed in (Zhang and Sarovar, 2014). For the two-qubit sensor, we employ the state space model obtained for a theoretical analysis and the Gröbner basis method in (Sone and Cappellaro, 2017) to demonstrate the numerical analysis. In this section, we briefly introduce the dynamical modeling of spin chain systems with a qubit sensor.

We consider a spin-\( \frac{1}{2} \) chain system consisting of \( N \) qubits with the Hamiltonian

\[
H = \sum_{m=1}^{N-1} h_m H_m,
\]

where the \( H_m \) are known Hermitian operators and the \( h_m \) are unknown coupling constants (strengths) to be estimated (Zhang and Sarovar, 2014). Considering that the magnitude of those unknown parameters is of most interest, the objective is to estimate the magnitudes \( \{|h_m|\} \) of these coupling strengths.

In this paper, we further specify the system to be the exchange model without transverse field (Franco et al., 2008; Christandl et al., 2005) whose Hamiltonian is

\[
H_k = \frac{h_k}{2} (X_k X_{k+1} + Y_k Y_{k+1}),
\]

where the subscript \( k \) indicates the \( k \)-th spin. To write the operators in a compact form, we omit the tensor product symbol and the identity operator unless otherwise specified.

Given the system Hamiltonian \( H \), the time evolution of an arbitrary system observable \( O(t) \) in the Heisenberg picture is

\[
\frac{dO(t)}{dt} = i[H, O(t)],
\]

where \( i = \sqrt{-1} \) is the imaginary unit and \( [A, B] = AB - BA \).

Let \( M \) be the measurement operator. Note that here we adopt a time trace measurement approach which involves taking average of measurements of a quantum system at a certain time for several runs under the same initial state. The average measurement value is then used as the expectation (Zhang and Sarovar, 2014).

The system operators that are coupled to \( M \), together with \( M \), form the accessible set \( G = \{O_1, O_2, O_3, \ldots\} \). See (Yu et al., 2019) for a detailed procedure of generating the accessible set.
Define the system state $x$ as the vector of all the expectations of the operators in the accessible set $G$ then we have
\[ x = [\hat{O}_1 \ \hat{O}_2 \ \cdots \ \hat{O}_i \ \cdots]^T \tag{11} \]
where $\hat{O}_i = \text{Tr}(O_i \rho)$ is the expectation value of observable $O_i \in G$. Intuitively, the elements in $G$ are those which are influenced by the measurement operator during the time evolution.

The linear equations describing the dynamics of the system can be written as
\[
\begin{align*}
  \dot{x} &= Ax, \\
  x(0) &= x_0.
\end{align*}
\tag{12}
\]
Given the system state $x$ defined in (11), the derivative of $x$ can be obtained using (10), based on which the $A$ matrix can then be calculated. Using the initial state of the system, the matrix $x_0$ is then determined. The matrix $C$ is obtained from the decomposition coefficients of the measurement matrix onto the operators in the state $x$. In (Zhang and Sarovar, 2014), the authors pointed out that a necessary condition for reconstructing the system is that all of the unknown parameters in $\{h_i\}$ appear in the matrix $A$.

The relationship between a transfer function and state space functions in (12) is
\[ G(s) = C(sI - A)^{-1}x_0, \tag{13} \]
where $s \in \mathbb{C}$ is the Laplace variable. Note that the relationship between the transfer function and the state space equations is not bijective, even up to a similarity transformation. There is a unique transfer function for a given state space matrix while there are many different state space realizations for a known transfer function.

The way that the sensor couples with the object system should be appropriately designed to effectively detect the information of interest. In this paper, we couple the sensor to the object system in the form of a string (See Figure 1) (Sone and Cappellaro, 2017; Wang et al., 2018).

### 2.3 Constraints on settings and the sensing capability

In practical situations, it can be difficult to initialize a qubit system to an arbitrary state or to measure the system using an arbitrary operator (e.g., in a solid-state qubit system). Special constraints may be applied for individual experiments. Here, we consider the case where the initial state can only be prepared in eigenstates of an $X$ operator (e.g., $|\psi_{\pm}\rangle$). In this paper, those constraints apply to both single- and two-qubit sensors.

The measurement capability of sensing qubits is essential. For example, we may be able to implement the measurement of $\sigma_z$ or $\sigma_x$ but not the measurement of $\sigma_y$. The measurement for a single-qubit sensor can be either $\sigma_z$ or $\sigma_x$; the measurement on a two-qubit sensor can be $I \otimes \sigma_z$, $I \otimes \sigma_x$, $\sigma_z \otimes \sigma_z$, $\sigma_z \otimes \sigma_x$, $\sigma_x \otimes \sigma_z$, or $\sigma_x \otimes \sigma_x$. The readout of the sensor provides us with information about the object system. These assumptions and constraints may come from practical engineering applications and constraints may be derived from the object system. We label the initial state of a qubit sensor in a specific state that can be reset and allow users to make specific measurements. However, our analysis is also applicable to other cases with different assumptions.

The sensing capability of a quantum sensor is defined in terms of whether the sensor can uniquely identify all of the unknown parameters $\{h_i\}$ in (9). If there is a bijective mapping between the unknown parameters and the data obtained from the sensor, then the sensor is capable of identifying all of the unknown coupling strengths. Thus, we consider the problem of determining if the mapping between the data and $\{h_i\}$ is bijective or not. In doing this, we do not consider any noise or uncertainty in the data.

For cases where the system is of an arbitrary dimension, the capability of the sensor can be analytically determined if we are given the state space model (Wang et al., 2018). Otherwise, given a fixed system dimension, we apply an approach involving transforming the state space model into its corresponding transfer function and then employing numerical methods to determine the unknown parameters (e.g., using the Gröbner basis method).

The capability of a sensor relates to the following aspects: the structure of the sensor and the object system, the measurement scheme and the initial settings. A good sensing scheme should ensure that all of the unknown parameters appear in the matrix $A$ with a proper structure and all of the parameters can be estimated given the measurement data. Here, we consider the capability of different sensing schemes for both a single-qubit sensor and a two-qubit sensor.

### 3. SINGLE-QUBIT SENSOR FOR SPIN CHAIN SYSTEMS

For a single-qubit sensor, an extra qubit is coupled to the object spin chain system which contains $N$ qubits. We label the sensing qubit with $\beta$ and the object qubits with natural numbers. Thus the total number of qubits in the system is $N + 1$.

For a single-qubit sensor applied to the system of (9), we have
\[ H = \frac{h_\beta}{2} (X_\beta X_1 + Y_\beta Y_1) + \sum_{k=1}^{N-1} \frac{h_k}{2} (X_k X_{k+1} + Y_k Y_{k+1}), \tag{14} \]
where $h_\beta (X_\beta X_1 + Y_\beta Y_1)$ is the interaction Hamiltonian indicating how the sensor and the chain system are coupled.

The initial state is
\[ \rho_{ini} = \rho_\beta^\|$,
\tag{15} \]
where $\rho_\beta^\|$ is the eigenstate of $X_\beta$. The superscript $x$ indicates the state is an eigenstate of the $X$ operator.

The two measurement schemes are $Y_\beta$ and $Z_\beta$. The corresponding accessible sets are listed below:

1) $M^1 = Y_\beta$,
   \[ G^1 = \{ Y_\beta, Z_\beta X_1, Z_\beta Z_1 Y_2, Z_\beta Z_1 Z_2 X_3, \cdots \}, \]
2) $M^2 = Z_\beta$,
   \[ G^2 = \{ Z_\beta, Y_\beta X_1, Y_\beta Y_1, Y_\beta Z_1 X_2, Y_\beta Z_1 Z_2, \cdots \}. \]

Note that we restrict the initial state to be prepared as eigenstates of the $X_\beta$ operator. However, $X_\beta$ belongs to neither the accessible set $G^1$ nor $G^2$, which means that the only available initial state $\rho_\beta^{ini}$ is orthogonal to all of the operators in their corresponding accessible sets. To put it differently, the operator $X_\beta$ is not coupled to any operators in the above accessible sets $G^1$ and $G^2$. In this situation, the expectations of the measurements $Y$ and $Z$ on the sensing spins are always zero which means that for both cases we have $x_0 = 0$. From (12), we always have $x \equiv 0$ which results in the measurement $y \equiv 0$ for both measurement schemes $M^1$ and $M^2$. Hence, no information can be extracted in these cases and the single-qubit sensor fails to identify the system Hamiltonian.
4. TWO-QUBIT SENSOR FOR SPIN CHAIN SYSTEMS

Since a single-qubit sensor is incapable of uniquely determining the unknown parameters of the spin chain system under the settings provided in Section 2.3, a new sensor is needed for this case. Our solution is to increase the number of qubits in the sensor and a measurement scheme for the two-qubit sensor is provided in this section which can perform the sensing task under the given settings.

4.1 Dynamical modeling

For a two-qubit sensor, two extra qubits are coupled to the object spin chain system in the form of a string. The Hamiltonian of the whole system is

\[
H = \frac{h_{\alpha}}{2} (X_\alpha X_\beta + Y_\alpha Y_\beta) + \frac{h_{\beta}}{2} (X_\beta X_1 + Y_\beta Y_1)
\]

\[+ \sum_{k=1}^{N-1} \frac{h_k}{2} (X_k X_{k+1} + Y_k Y_{k+1}), \tag{16}\]

where \(\frac{h_{\alpha}}{2} (X_\alpha X_\beta + Y_\alpha Y_\beta)\) is the internal Hamiltonian of the two spins of the qubit sensor while \(\frac{h_{\beta}}{2} (X_\beta X_1 + Y_\beta Y_1)\) is the interaction Hamiltonian of the sensor and the chain system. The subscripts \(\alpha\) and \(\beta\) indicate the first and second spins of the sensor, respectively. \(h_{\alpha}\) can be fabricated and we assume that it is known to us while \(h_{\beta}\) could be either unknown or known. The sensor is employed to identify all of the unknown parameters in \(\{|h_i|\}\).

The initial state of the two-qubit sensor is chosen as \(|\frac{1}{2} \otimes \rho_\beta\).

4.2 Capability test when measuring \(Y_\alpha Z_\beta\)

Numerical results show that for an arbitrary \(N\), the state space model given in (19), (20) and (21) may not be minimal. The mapping between the measurement data and a non-minimal state space model is not bijective. Thus a minimal realization is required. However, the dimension of the state space model in this case increases rapidly at the scale of \(O(N^3)\) while the corresponding minimal system has a much lower dimension.

Thus the structure of the state space model is dramatically changed when obtaining its minimal system. As a result, there is not a clear repetition pattern in the structure of the minimal state space model, although the original non-minimal model has a good repetition structure with increasing \(N\). The unclear structure of the minimal state space model makes it difficult to have an analytic result which applies for any spin number \(N\). Here, we leave the sensing capability testing problem for an arbitrary \(N\) as an open problem and provide readers with a numerical method, the Gröbner basis method (Sone and Cappellaro, 2017).

The main idea of the Gröbner basis method is that: for a given state space model, one can obtain the system transfer function \(G(s)\) with unknown parameters using (13). On the other hand, one can also reconstruct a system transfer function \(\hat{G}(s)\) from the measurement data using the ERA method (Zhang and Sarovar, 2014). Since the two transfer functions describe the same input-output behavior, we have

\[\hat{G}(s) = G(s)\].

By equating the coefficients in (22), a polynomial set \(F\) with respect to unknown parameters in \(\{|h_i|\}\) can be obtained. The unknown parameters \(\{|h_i|\}\) can then be inferred by solving the polynomial set \(F\). The sensing capability is then related to the number of the solutions of \(F\). If the solution of \(F\) is unique, the parameters are identifiable.

The Gröbner basis method is a widely used algorithmic solution for a set of multivariate polynomials (Buchberger, 2001). Details of the algorithm to test identifiability is given in (Sone and Cappellaro, 2017). As an example, we illustrate the use of the Gröbner basis method for testing the capability of a two-qubit quantum sensor when \(N = 2\).

The Hamiltonian for the system (16) when \(N = 2\) is

\[
H = \frac{h_{\alpha}}{2} (X_\alpha X_\beta + Y_\alpha Y_\beta) + \frac{h_{\beta}}{2} (X_\beta X_1 + Y_\beta Y_1)
\]

\[+ \frac{h_1}{2} (X_1 X_2 + Y_1 Y_2). \tag{23}\]

The corresponding matrices for the state space model are given in (19), (20) and (21). We have

\[x_0 = [0 \ 1 \ 0 \ 0 \ 0 \ldots]^T \tag{20}\]

and

\[C = [1 \ 0 \ 0 \ 0 \ 0 \ldots]. \tag{21}\]

Note that the matrix \(A\) is a sparse matrix and has a special repetition pattern.
\[ G(s) = C(sI - A)^{-1}x_0 = -h_\alpha s^{10} + (10h_3^\alpha + 7h_\alpha h_2^\beta + 11h_\alpha h_1^\beta) s^8 + \cdots \]

We sort the numerator and the denominator of the transfer function by the order of \( s \) and only present items of the highest and second highest order. The residual terms of lower order are omitted since the first two terms are sufficient for determining the sensor capability. Moreover, we assume that the transfer function obtained by the measurement data is

\[ \hat{G}(s) = -v_1 s^{10} + v_2 s^8 + \cdots \frac{1}{s^{12} + v_3 s^{10} + \cdots} \]

where \( v_1, v_2, v_3, \ldots \) are real values obtained from the ERA method (Zhang and Sarovar, 2014). From (22), we have the following equation

\[ h_\alpha s^{10} + (10h_3^\alpha + 7h_\alpha h_2^\beta + 11h_\alpha h_1^\beta) s^8 + \cdots \]

\[ \frac{1}{s^{12} + 11(h_2^\alpha + h_2^\beta + h_1^\beta) s^{10} + \cdots} \]

We substitute the variables by \( \theta_1 = h_\alpha, \theta_2 = h_2^\alpha, \theta_3 = h_2^\beta \) since we are only concerned with the amplitudes \( \{ |h_i| \} \). Equating the coefficients in (25) and (26), we have \( \theta_1 = v_1, 10\theta_2 \theta_3 + 11 \theta_1 \theta_2 + 11 \theta_2 \theta_3 = v_2, 11(\theta_2^2 + \theta_2 + \theta_3) = v_3 \). The Gröbner basis of these polynomials takes the following form:

\[ \mathcal{G} = \{ \theta_1 - a_1, \theta_2 - a_2, \theta_3 - a_3 \} \]

where \( a_1 = v_1, a_2 = -v_3 + v_1 v_3 - v_2 / (4v_1), a_3 = -3v_3^2 - 7v_1 v_3 + 11v_1 / (44v_1) \). It can be seen that there is only one solution for the magnitudes of all of the parameters. Therefore, the sensor is capable of identifying these parameters.

We conclude that the two-qubit sensor is capable of identifying all of the unknown parameter amplitudes \( \{ |h_i| \} \) in the system (9) when \( N = 2 \). Moreover, for any given \( N \), the capability can also be confirmed by the Gröbner basis method (Yu et al., 2020).

5. CONCLUSION

We have investigated the capability of a class of qubit sensors. The object system is a spin chain system whose Hamiltonian is given with unknown coupling parameters. Qubit sensors are coupled to the object system in order to achieve parameter identification. By initializing and probing the qubit sensor, our aim is to estimate all of the unknown parameters. The objective of this paper is to determine whether certain proposed sensing schemes can successfully achieve the sensing task. We compare the sensing capability of single- and two-qubit sensors subject to restricted initial settings and measurement schemes. We find that a single-qubit sensor is not capable of fully performing the estimation task under the specified settings. To solve this problem, we propose the use of two-qubit sensors and provide a case where a two-qubit sensor can estimate all of the unknown parameters, which reveals an effective way to improve the capability of quantum sensors through increasing the number of qubits in the sensor.

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