Stochastic parameter-shift rule for quantum metrology with general Hamiltonians

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ABSTRACT

Recently, quantum metrology with multiplicative Hamiltonians has been proposed in the variational quantum algorithms, from which the estimation precision can be adaptively optimized via the variational circuits. For systems with general Hamiltonians, however, still lack these variational schemes. In this work, we introduce a quantum-circuit-based approach for studying quantum metrology with general Hamiltonians. We introduce the stochastic parameter-shift rule for the derivatives of the evolved quantum state under the parameterized gates in the circuit, whereby the quantum Fisher information can be obtained. Here the parameters are those we wish to estimate. We find that under the family of the parameterized gates, our scheme can be executed in universal quantum computers. Moreover, in the examples of the magnetic field estimation, we show the consistency between the results obtained from the stochastic parameter-shift rule and the exact results while the standard parameter-shift rule slightly deviates from the exact ones. Our work sheds new light for studying quantum metrology with general Hamiltonians using quantum circuit algorithms.

Introduction

The objective of quantum metrology is that using nonclassical quantum resources, including entanglement and squeezing, to enhance the precision in the estimation of unknown parameters. It has a wide range of applications from quantum magnetometry, quantum clock, quantum imaging, gravitational-wave detection, dark matter detection, and so on. So far, it has been demonstrated the quantum-enhanced precision beyond the Heisenberg limit with nonlinear interaction, interaction-based, and even without entanglement. The studies of quantum metrology under noisy environments, post-selection measurements, and quantum error correction are also extensively reported.

The cornerstone of quantum metrology is the quantum estimation theory, in which it imposes the ultimate lower bound for the precision of any estimator by a quantum counterpart of the Cramér-Rao inequality. That quantum Cramér-Rao bound is associated with the quantum Fisher information (QFI), for single-parameter estimation or quantum Fisher information matrix (QFIM, for multiparameter estimation), the maximum information that we can gain from the measured system.

Numerous previous studies on quantum metrology mainly focused on the overall multiplicative parameters of Hamiltonians. However, recent attentions have been raised to general parameters of Hamiltonians, such as quantum magnetometry, unitary parametrization process, time-dependent Hamiltonians. While the estimation with general Hamiltonians shares some typical characteristics as the estimation with multiplicative parameters of Hamiltonians, it likewise indicates other distinct features, such as getting high efficiency with time scaling and with quantum control. The study of the ultimate quantum bounds in these general cases is thus appealing so that it could open a broad range of potential applications in quantum metrology and even quantum computing.

Quantum computers can outperform classical ones and open significant advantages for exponentially speeding up various computational tasks. Specifically, the birth of Noisy Intermediate-Scale Quantum (NISQ) computers results in the brilliant growth of various quantum algorithms (see the reviews). Among them, the variational quantum algorithms are the most widely studied as a promising approach for improving efficiency in the noisy and few-qubits devices, including variational quantum eigensolvers, quantum approximate optimization algorithms, new frontiers in quantum foundations, and so on (see the review). Besides, many computational tools based on variational quantum circuits have been developed, including the standard parameter-shift rule (Stand.PSR) and quantum natural gradient (QNG). The Stand.PSR is a method that allows us to get the exact partial derivatives of any function by calculating the parameter-shift in the circuits. Suppose we have a quantum circuit function \( f(x) \) as the expectation value of an observable \( A \):

\[
\langle A \rangle = \langle \psi | U(x) A U(x)^\dagger | \psi \rangle,
\]

where the evolution

\[
U(x) = \prod_j U_j(x)
\]

contains a sequence of parameterized gates

\[
U_j(x) = e^{-i x H_j}
\]

with the Hermitian generator \( H_j \), and \( | \psi \rangle \) is the initial state of the circuit. The Stand.PSR allows for evaluating the exact gradient \( \partial_x f(x) \) that proportional to the linear combination in the expectation values of the same circuit with different shifted parameters

\[
\partial_x f(x) = r [ f(x + \mu) - f(x - \mu) ]
\]

where the relationship between the multiplier \( r \) and the shifted \( \mu \) depend on the quantum gate \( U(x) \) of the circuit.

However, it can be seen that the Stand.PSR is only applicable for cases whose the generators \( H_j \) commute with each other or whose parameterized gates \( U_j(x) \) are uncorrelated. In general cases, to apply the Stand.PSR, it requires additional treatments such as the Hamiltonian simulation technique. Recently, Banchi and Crooks in their seminal work have developed a stochastic parameter-shift rule (Stoc.PSR) for the general quantum evolutions. Their approach relies on the stochastic repetitions of quantum measurement and thus does not need any extra solution.

So far, different variational quantum algorithms for quantum
with multiplicative parameters of Hamiltonians. In this way, a quantum state is generated using the variational parameters that will be updated gradually to get a proper quantum resource for metrology. Thus, it requires developing novel approaches to evaluate the estimation precision directly in quantum circuits. While the Stand.PSR had been widely utilized in various aspects, including fitting the QFI with multiplicative parameters of Hamiltonians\(^{17-33}\), it is lacking for the study of general Hamiltonians. Nevertheless, in reality, many systems are governed by the general Hamiltonians. So that, the current studies on quantum metrology with multiplicative parameters of Hamiltonians will extremely limit the applications and thus, the study of general Hamiltonians using quantum algorithms is urgent for allowing the application of quantum metrology in more general situations.

This article fills the urgent demand by presenting a general form for the Stoc.PSR and apply it to quantum metrology to derive the QFIM (or QFI) and hence examine the estimation precision. We apply the proposed Stoc.PSR for the derivatives of the evolved quantum state under the sensing parameterized gates, from which the QFIM is obtained. Here the parameters are those we wish to estimate. We find that under the family of the sensing parameterized gates, our scheme can be executed in a universal quantum computer. In the examples of the magnetic field estimation, we show that the results obtained from the Stoc.PSR agree with the exact results while the Stand.PSR’s results deviate from the exact values. This observation suggests the meaning and importance of the Stoc.PSR in quantum circuit algorithms for studying quantum metrology with general Hamiltonians.

**Results**

**Quantum parameters estimation for general Hamiltonians**

Estimation is a measurement process performed on an interested system to extract its information by coupling with a probe. Given the system with \(d\) unknown parameters in a field \(B = \phi_1 e_1 + \cdots + \phi_d e_d\), where \(e_j\) are unit vectors in \(j\) directions, the interaction imprints the field’s information into the probe via \(H(\phi) = B \cdot H = \sum_{j=1}^d \phi_j H_j\). Here, \(H(\phi)\) is a general Hamiltonian, where all \(H_j\) do not commute with each other. The task of quantum parameters estimation is to evaluate these unknown coefficients by measuring the probe.

Given the initial probe state \(\rho_0\), after the interaction, it evolves to \(\rho(\phi) = U(\phi)\rho_0 U^\dagger(\phi)\), where \(U(\phi) = e^{-itH(\phi)}\) represents the unitary evolution during the interaction time \(t\). When the probe state is measured, the probabilities distribution reveals the parameters’ information. Measure in a general basis set, i.e., the positive operator-values measure (POVM) \(\{E_x\}\) for the outcomes \(x\), the corresponding probabilities read \(p(x|\phi) = \text{tr}[\rho(\phi)E_x]\), from which \(\phi\) can be estimated.

In the estimation theory, the estimated values \(\hat{\phi}(x)\) are obtained by a certain estimator wherein different estimator strategies, such as maximum-likelihood estimation\(^{74,75}\), least square\(^{76}\), may yield different precision. The estimation precision can be characterized in terms of covariance matrix\(^{35}\)

\[
C(\phi) = E\left[\left(\phi - E[\phi(x)]\right)\left(\phi - E[\phi(x)]\right)^T\right], \quad \text{where } E[\hat{X}] = \int p(x|\hat{X})\hat{X}(x)dx \text{ is the expectation value of the estimator } \hat{X}(x).
\]

The diagonal terms \(C_{k,k} = \Delta^2\phi_k = E[\phi_k^2] - E^2[\phi_k]\) are the variances for estimating \(\phi_k\), and the off-diagonal terms \(C_{k,l}\) are the covariances between \(\phi_k\) and \(\phi_l\). An estimator is unbiased when \(E[\phi_k(x)] = \phi_k, \forall k \in \{1, \cdots, d\}\). In general, the precision limit for an arbitrary estimator strategy is given by classical and quantum Cramér-Rao bounds (CRBs)\(^{36-41}\), in which state that

\[
MC(\phi) \geq F^{-1}(\phi) \geq Q^{-1}(\phi),
\]

where \(M\) the repeated measurements, \(F(\phi)\) is the classical Fisher information matrix (CFIM) defined as\(^{41}\)

\[
F_{k,l} = \int p(x|\phi)\left[\partial_{\phi_k} \ln p(x|\phi)\right]\left[\partial_{\phi_l} \ln p(x|\phi)\right]dx,
\]

and maximize all possible measurements \(\{E_x\}\) yields the quantum Fisher information matrix (QFIM) \(Q(\phi)\) as\(^{77,78}\)

\[
Q_{k,l} = \text{tr}\left[L_k L_l \rho(\phi)\right],
\]

where \(2\partial_{\phi_k}\rho(\phi) = L_k \rho(\phi) + \rho(\phi)L_k\) is the standard logarithmic derivative (SLD)\(^{79}\). Mentioning that both the CFIM and QFIM may depend on the parameters \(\phi\) regardless of the unitary process. For a single parameter (such as \(\phi\)) estimation, the CRBs simplify \(\Delta^2\phi \geq 1/F(\phi) \geq 1/Q(\phi)\), where \(F(\phi) = \int p(x|\phi)\left[\partial_{\phi} \ln p(x|\phi)\right]^2dx\), and \(Q(\phi) = \text{tr}[L^2 \rho(\phi)]\), the classical and quantum Fisher information, respectively.

Quantum Fisher information (QFI) and quantum Fisher information matrix (QFIM) set the ultimate bounds for the estimation precision of any estimator strategy. It is thus important to derive these QFI and QFIM for the estimation theory with general Hamiltonian parameters. Let us start with the derivative of the unitary evolution\(^{10,42,80}\)

\[
\frac{\partial e^{-itH(\phi)}}{\partial \phi_j} = -i\int_0^t e^{-i\bar{s}H(\phi)}\left[\partial_{\phi_j} H(\phi)\right] e^{-i(t-s)H(\phi)}ds,
\]

\[
= -iU(\phi)Y_j,
\]

where \(Y_j = \int_0^t e^{-i\bar{s}H(\phi)}\left[\partial_{\phi_j} H(\phi)\right] e^{i\bar{s}H(\phi)}ds\) are Hermitian operators\(^{10,42,80}\). Then, we obtain

\[
\frac{\partial \rho(\phi)}{\partial \phi_j} = iU(\phi)\left[\rho_0, Y_j\right]U^\dagger(\phi).
\]

The QFIM (3) straightforwardly yields

\[
Q_{k,l} = 2 \sum_{p,\mu,\nu > 0} \frac{\langle \lambda|\partial_{\phi_k} \rho(\phi)|\lambda\rangle \langle \mu|\partial_{\phi_l} \rho(\phi)|\mu\rangle}{p_{\lambda} + p_{\nu}},
\]

for \(\rho(\phi) = \sum_{\lambda} p_{\lambda} |\lambda\rangle\langle \lambda|\), and \(\partial_{\phi_k;i\lambda}\rho(\phi)\) are given from Eq. (5). An alternative way to derive the QFIM was proposed in Ref.\(^{81}\) using the vectorization method

\[
Q_{k,l} = 2 \text{vec}[\partial_{\phi_k} \rho(\phi)]^\dagger [\rho(\phi) \otimes I + I \otimes \rho(\phi)]^{-1} \text{vec}[\partial_{\phi_l} \rho(\phi)],
\]

where \(\text{vec}[A] = \sum_{j=1}^n e_j \otimes Ae_j\) is a column vector formed from an \(n \times n\) matrix \(A\), and \(\rho(\phi)\) is the complex conjugate of \(\rho(\phi)\).
For pure quantum states, i.e., \( \rho_0 = |\psi_0\rangle\langle\psi_0| \), the QFIM is defined by\(^{82}\)
\[
Q_{k,l} = 4\text{Re} \left[ \langle \partial_{\phi_k} \psi(\phi) | \partial_{\phi_l} \psi(\phi) \rangle - \langle \partial_{\phi_l} \psi(\phi) | \partial_{\phi_k} \psi(\phi) \rangle \langle \psi(\phi) | \partial_{\phi_l} \psi(\phi) \rangle \right]. \tag{8}
\]
where \( |\psi(\phi)\rangle = U(\phi)|\psi_0\rangle \) the evolved probe state. Apply Eq. (4), it yields\(^{10,44}\)
\[
Q_{k,l} = 4\text{Re} \left[ \langle \psi_0 | Y_k Y_l | \psi_0 \rangle - \langle \psi_0 | Y_l | \psi_0 \rangle \langle \psi_0 | Y_k | \psi_0 \rangle \right]. \tag{9}
\]
Admitted that these methods for QFIM (and similar for QFI) reply on the derivatives of the probe state, i.e., \( \partial_{\phi_j} \rho(\phi), \forall j \in \{1, \cdots, d\} \). Hereafter, we introduce a stochastic parameter-shift rule (Stoc.PSR) to compute these derivatives on quantum circuits, and thus, the estimation precision can be evaluated in various quantum computer platforms.

**Stochastic parameter-shift rule**

In this section, we provide the stochastic parameter-shift rule (Stoc.PSR) for quantum metrology with general Hamiltonians, where we particularly calculate \( \partial_{\phi_j} \rho(\phi) \) in quantum circuits. This method is thus helpful for studying different variational quantum algorithms\(^{55}\), including variational quantum metrology\(^{64,65}\) and evaluating Fubini-Study metric tensor in quantum natural gradient\(^{58}\).

First, we recast the quantum probe state as
\[
\rho(\phi) = e^{Z} [\rho_0],
\]
where \( Z = -it \sum_j \phi_j H_j \) and the superoperator \( e^{Z} [\rho_0] = e^Z \rho_0 e^{-Z} \). Let \( Z[\rho_0] = [ -it \sum_j \phi_j H_j, \rho_0 ] \) is a superoperator, and \( V = \partial_{\phi_j} Z = -it[H_j, \rho_0] \). Then, for \( H_j = I \), we derive
\[
\frac{\partial Z[\rho_0]}{\partial \phi_j} = e^{-it \mu H_j} \rho_0 e^{it \mu H_j} - e^{it \mu H_j} \rho_0 e^{-it \mu H_j}. \tag{11}
\]
Recall that in ref.\(^{70}\) the framework fixes \( \mu = \pi/4 \) and \( t = 1 \), here we consider any time \( t \) and introduce \( \mu \) an arbitrary parameter-shift, which makes our scheme more general. Finally, from the first line Eq. (4) and Eq. (11), the derivative \( \partial_{\phi_j} \rho(\phi) \) yields
\[
\frac{\partial \rho(\phi)}{\partial \phi_j} = \frac{1}{2 \sin (t \mu)} \int_0^t \left[ \rho^+_j(\phi, s) - \rho^-_j(\phi, s) \right] ds, \tag{12}
\]
we call the stochastic parameter-shift rule (Stoc.PSR), where
\[
\rho^+_j(\phi, s) = U^+_j(\phi, s) \rho_0 U^+_j(\phi, s)^\dagger, \tag{13}
\]
\[
U^+_j(\phi, s) = e^{-isH(\phi)} e^{it \mu [\delta_{\phi_j} H(\phi)]} e^{-i(t-s)H(\phi)}. \tag{14}
\]

The algorithm for Stoc.PSR is described in Algorithm 1.

Figure 1 depicts a quantum circuit for the Stoc.PSR. For every given time \( t \), we process the following steps to derive \( \partial_{\phi_j} \rho(\phi) \) in the circuit and get the corresponding \( Q(\phi) \): (s1) generate a random number \( s \) follows the normal distribution in an interval \([0, 1]\); (s2) prepare an initial state \( \rho_0 \) in the quantum circuit; (s3) apply a sequence of quantum gates \( e^{-it(t-s)H(\phi)}, e^{-it \mu [\delta_{\phi_j} H(\phi)]}, \) and \( e^{-isH(\phi)} \) onto the circuit; (s4) extract the final quantum state \( \rho^+ \) from the circuit; (s5) repeat steps s2-s4 where the gate \( e^{-it \mu [\delta_{\phi_j} H(\phi)]} \) in s3 is replaced by \( e^{-it \mu [\delta_{\phi_j} H(\phi)]} \) and in s4, the quantum state assigns to \( \rho^+ \); (s6) repeat steps s1-s5 \( N \) times and compute the derivative \( \partial_{\phi_j} \rho(\phi) \) via
\[
\frac{1}{N} \sum_{n=1}^N (\rho^+ - \rho^-) \text{ comes from Eq. (12), where } t/N \text{ is the average in Monte-Carlo sampling.}
\]

**Algorithm 1: Stochastic parameter-shift rule**

**Data:** \( \rho_0, \phi = (\phi_1, \cdots, \phi_d), H(\phi) = \sum_j \phi_j H_j \)

**Result:** \( Q(\phi) \)

\[ T \leftarrow \text{time (array)}; \]
\[ N \leftarrow \text{sampling number}; \]
\[ \mu \leftarrow \text{parameter-shift(\text{rad})}; \]
\[ \text{for } t \in T \text{ do } \]
\[ \text{for } j = 1, \cdots, d \text{ do } \]
\[ s = \text{random}(0, 1) \]
\[ \text{get } U^+_j(\phi, s) \]
\[ \text{get } \rho^+_j(\phi, s) \]
\[ \text{get } \partial_j = \rho^+_j(\phi, s) - \rho^-_j(\phi, s) \]
\[ \text{end} \]
\[ \text{end} \]
\[ \text{compute } Q(\phi) \text{ from Eq. (6) or (7) or (8)}. \]

**Applications**

To demonstrate the advantages feature of our Stoc.PSR method for quantum metrology, we scrutinize the estimation in two cases of single and multiple magnetic fields as follows.

**Single parameter estimation**

Let us consider a magnetic field \( B = \cos(\phi) e_x + \sin(\phi) e_z \), and we want to estimate the angle \( \phi \) between the field’s direction and the \( z \) axis\(^{12}\). The field interacts with an exposed qubit probe and imprints its information into the probe via the interaction
where

\[ Q(\phi) = 4\text{Re}\left[ \langle \psi_0 | Y^2 | \psi_0 \rangle - |\langle \psi_0 | Y | \psi_0 \rangle|^2 \right] = 4\sin^2(t) \left[ 1 - \cos^2(t) \sin^2(\phi) \right], \]

(16)

where \( Y_\phi = \int_t^0 e^{-i\phi H(\phi)} \partial_\phi H(\phi) e^{i\phi H(\phi)} \, dx \). It can be observed that \( Q(\phi) \) varies with the interaction time \( t \) and reaches its maximum of 4 at \( t = \pi/2 \) as seen from the solid curves in figure 2.

This behavior comes from the fact that the probe state rotates in time under the effect of the magnetic field, which results in the oscillation of the variance. Furthermore, the QFI depends on the true parameter value, thus it becomes a function of \( \phi \). In the limit \( \phi \to 0 \), the QFI yields \( Q(\phi) = Q_{\text{max}} = 4\sin^2(t) \).

We now process the Stoc.PSR. Consider a quantum circuit with a single qubit initially prepared in \( |0\rangle \) and becomes \( |\psi_0\rangle \) after applying a Hadamard gate. Following algorithm 1, we derive \( |\psi^+\rangle \) in the circuit as

\[ |\psi^+\rangle = U(s, \phi) \cdot e^{\mp i\mu \partial_\phi H(\phi)} \cdot U(t - s, \phi) |\psi_0\rangle, \]

(17)

where \( s \in [0, t] \) is a random sampling, and \( \mu \) is arbitrary. The derivative \( \partial_\phi |\psi(\phi)\rangle = \frac{N^2}{\lambda^2 \sin(t\mu)} \sum_{n=1}^N [ |\psi^+\rangle - |\psi^-\rangle ] \) is obtained after \( N \) samplings. In the numerical calculation, we set \( N = 1000 \) and \( \mu = \pi/3 \) and obtain the QFI \( Q(\phi) \) which is of the form (8)

\[ Q(\phi) = \frac{t^2}{N^2 \sin^2(t\mu)} \text{Re} \left[ \langle \Psi | \Psi \rangle - |\langle \Psi | \psi(\phi) \rangle|^2 \right], \]

(18)

where \( |\Psi\rangle = \sum_{n=1}^N [ |\psi^+\rangle - |\psi^-\rangle ] \).

To implement the Stoc.PSR in quantum computers, we assume there exists a universal quantum hardware that allows for executing a quantum gate \( U(t, \phi) \). Changing the variables in \( U(t, \phi) \) by \( U(x, z) = e^{-it(x\sigma_x + z\sigma_z)} \) where \( x = \cos(\phi) \) and \( z = \sin(\phi) \), it yields \( \partial_\phi U(x, z) = \partial_x U(x, z) \partial_\phi x + \partial_z U(x, z) \partial_\phi z \). It is thus a universal quantum device because all the evolution terms in Eq. (17) can be implemented via this quantum gate in the device.

Finally, let us compare the results with the Stand.PSR. To apply the Stand.PSR, we decompose the evolution \( U(t, \phi) \) into a sequence of sub-evolutions through Trotter-Suzuki transformation as

\[ U(t, \phi) = \lim_{m \to \infty} \left( e^{-it \cos(\phi) \sigma_x / m} e^{-it \sin(\phi) \sigma_z / m} \right)^m. \]

(19)

Here, these sub-evolutions can be executed in quantum circuits by rotation gates, i.e., \( R_x \) and \( R_z \). The derivative \( \partial_\phi |\psi(\phi)\rangle \) is thus can be implemented using the Stand.PSR. See detailed calculation in the Method.

In figure 2, we compare the performance of the Stand.PSR and Stoc.PSR with the exact theoretical result. The Stoc.PSR displays a good agreement with the exact results for all the time while the Stand.PSR deviates from the exact results when increasing the interaction time. It implies that using Stoc.PSR in quantum circuits for studying quantum systems with general Hamiltonian is essential and may not be replaced by similar approximation methods.
We show the exact theoretical results by solid curves for different choices of \( \varphi \) as shown in the figure. Here, we use \( \varphi_x = \varphi_y = \varphi_z = \varphi \) for the sake of illustration (in general, they may be different). The solid curves are exact results given by theoretical analysis, and the dotted curves are obtained from the Stoc.PSR. It can be observed that \( \text{tr}[Q^{-1}] \) varies with the time \( t \) and reaches its minimum at a certain time. More importantly, the results show a good agreement between the Stoc.PSR and the exact theoretical analysis.

### Multiple parameters estimation

We now turn to apply our Stoc.PSR scheme for estimating the components of a magnetic field pointing in an arbitrary direction. Consider the probe state initially prepared in \( n \)-qubit GHZ state \( |\psi_0\rangle = (|00\cdots0\rangle + |11\cdots1\rangle)/\sqrt{2} \), such that allows for obtaining the maximum QFIM \(^7\). The interaction Hamiltonian is given by

\[
H(\phi) = \sum_j \phi_j J_j, \quad \text{for} \quad j \in \{x,y,z\}. \quad (20)
\]

Here, \( \phi = (\phi_x, \phi_y, \phi_z) \) are the three components of the given magnetic field that we want to estimate, and \( J_j = \sum_{k=1}^n \sigma_j^{(k)} \) are the collective Pauli matrices. Potential platforms for the probe include spin-1/2 ensemble semiconductors, ions traps, NMR systems, and NV centers\(^{86-90}\). In these systems, such as spin-1/2 ensemble, \( J_j \) become the collective angular momentum operators\(^{10}\).

The QFIM can be obtained theoretically from equation (9), and the total variance yields \( \Delta^2 \phi = \text{tr}[Q^{-1}] \). Concretely, for a fix \( n = 3 \) qubits and \( \phi_x = \phi_y = \phi_z = \varphi \), we obtain

\[
\text{tr}[Q^{-1}] = \frac{7}{108 \varphi^2} + \frac{3 \varphi^2}{54 \sin^2(\sqrt{3} \varphi t)}. \quad (21)
\]

We show the exact theoretical results by solid curves for different \( \varphi \) in figure 3. It can be seen that for each \( \varphi \), there is a minimum variance at a certain time \( t \). Again, this result is caused by the rotation of the probe state under the effect of the magnetic field. In the limit of the small phase, i.e., \( \varphi \to 0 \), then \( \text{tr}[Q^{-1}] = \frac{7}{108 \varphi^2} \) which results in the minimum of the total variance.

In the Stoc.PSR method, we model the probe in an \( n \)-qubit quantum circuit initially prepared in the GHZ state. The circuit can be implemented in the existing noisy intermediate-scale quantum (NISQ) computers\(^{52}\). Its state evolves under the transformation \( U(t, \phi) = e^{-iH(\phi) t} \), and results in the evolved state \( |\psi(\phi)\rangle = U(t, \phi)|\psi_0\rangle \). As discussed above, this unitary evolution can be implemented in a universal quantum computer. Therefore, we employ the Stoc.PSR using algorithm 1 to obtain \( \Delta \phi_j |\psi(\phi)\rangle \) for all \( j \) and get the QFIM as in Eq. (8). The \( \text{tr}[Q^{-1}] \) is shown in figure 3 (dotted curves) for the number of sampling \( N = 1000 \). Again, in this case, the Stoc.PSR’s results agree with the exact results.

### Discussion

We proposed a stochastic parameter-shift rule (Stoc.PSR) framework for deriving the differential in the study of quantum metrology with general Hamiltonian generators. Our method allows for obtaining the exact derivative using universal quantum circuits, from which the quantum Fisher information can be derived. Different from the standard parameter-shift rule (Stand.PSR), which particularly relies on commuting Hamiltonians as quantum generators in quantum gates, here, the Stoc.PSR applies for general Hamiltonians.

Within our derived general scheme for the Stoc.PSR, the estimation of single and multiple parameters can be practically executed in quantum circuits. In all cases of the demonstration, the results from the Stoc.PSR always consent with the exact theoretical analysis while the Stand.PSR’s results deviates from that exact values.

Our results highlight an important practical aspect for quantum metrology with quantum algorithms computing. While the variational quantum algorithms are extensively developing, our framework has used these advantages for the development of quantum metrology and quantum measurement in general and makes them reliable for studying in the area of quantum computers.

### Methods

#### Theoretical analysis

First, let us discuss an exact calculation method for quantum Fisher information in single parameter estimation. Starting from \( H(\phi) = \cos(\phi)\sigma_x + \sin(\phi)\sigma_z \), we derive \( \partial_\phi H(\phi) = -\sin(\phi)\sigma_x + \cos(\phi)\sigma_z \). Substituting this into \( Y_j \) for \( j = \phi \), we obtain

\[
Y_\phi = \int_0^t e^{-i s H(\phi)} \left[ \partial_\phi H(\phi) \right] e^{i s H(\phi)} ds = \frac{1}{2} \begin{pmatrix}
\sin 2t \cos \phi & -\sin 2t \sin \phi + 2t \sin^2 t \\
-\sin 2t \sin \phi - 2t \sin^2 t & -\sin 2t \cos \phi
\end{pmatrix}.
\]

Finally, we derive the quantum Fisher information as in Eq. (8):

\[
Q(\phi) = 4 \text{Re}\left[ \langle \psi_0 | Y_\phi^2 | \psi_0 \rangle - \langle \psi_0 | Y_\phi | \psi_0 \rangle^2 \right] = 4 \sin^2(t) \left[ 1 - \cos^2(t) \sin^2(\phi) \right], \quad (22)
\]

which results in Eq. (16).
Hereafter, we derive for the multiple parameters estimation. For \( n = 3 \), we first calculate \( J_j \) for \( j = \{x, y, z\} \) as

\[
J_j = \sigma_j \otimes I_2 \otimes I_2 + I_2 \otimes \sigma_j \otimes I_2 + I_2 \otimes I_2 \otimes \sigma_j,
\]

where \( I_2 \) is the \( 2 \times 2 \) identity matrix. The Hamiltonian \( H(\phi) \) is given in Eq. (20) and its derivative yields \( \partial_\phi H(\phi) = J_j \). Similar to above, we derive \( Y_j \)

\[
Y_j = \int_0^t e^{-isH(\phi)} J_j e^{isH(\phi)} ds,
\]

and obtain the quantum Fisher information matrix from Eq. (9).

**Trotter-Suzuki transformation and Stand.PSR.** From now on, let us show the detailed calculation for the Trotter-Suzuki transformation and Stand.PSR for single parameter estimation. From the evolution (19), we set

\[
\begin{align*}
x &= \frac{2m}{\pi} \cos(\phi) \\
z &= \frac{2m}{\pi} \sin(\phi)
\end{align*}
\]

Then, Eq. (19) is recast as

\[
U(x, z) = \lim_{m \to \infty} \left( e^{-i\frac{\phi}{m} \sigma_z} e^{-i\frac{\phi}{m} \sigma_z} \right)^m,
\]

and thus

\[
\partial_\phi U(x, z) = \frac{\partial U(x, z)}{\partial x} \frac{\partial x}{\partial \phi} + \frac{\partial U(x, z)}{\partial z} \frac{\partial z}{\partial \phi}.
\]

Concretely, we have

\[
\begin{align*}
\partial_x U(x, z) &= \frac{m}{2} (-i\sigma_x) U(x, z) = \frac{m}{2} U(x + \pi, z), \\
\partial_z U(x, z) &= \frac{m}{2} (-i\sigma_z) U(x, z) = \frac{m}{2} U(x, z + \pi).
\end{align*}
\]

Here, we have used \( U(\pi, 0) = (-i\sigma_x)^m \) and chosen \( m = 4k + 1 \forall k \in \mathbb{N} \), so that \( U(\pi, 0) = -i\sigma_x \). Likewise, \( U(0, z + \pi) = -i\sigma_z \). In our calculation, we have chosen \( m = 401 \). Hence, these derivatives (28, 29) can be obtained in quantum circuits by modifying the Stand.PRS.

Substituting Eqs. (28, 29) and Eq. (25) into Eq. (27), we derive

\[
\partial_\phi |\psi_0(\phi)\rangle = \partial_\phi U(x, z) |\psi_0(\phi)\rangle
 = t \left[ -\sin(\phi) U(x + \pi, z) + \cos(\phi) U(x, z + \pi) \right] |\psi_0(\phi)\rangle,
\]

where \( |\psi_0(\phi)\rangle \) is the initial probe state. In this form, the QFI is given as

\[
Q(\phi) = 4 \text{Re} \left[ \langle \partial_\phi \psi_0(\phi) | \partial_\phi \psi_0(\phi) \rangle - |\langle \partial_\phi \psi_0(\phi) | \psi_0(\phi) \rangle|^2 \right].
\]

The procedure for calculating the quantum Fisher information is shown in algorithm 2 below.

---

**Algorithm 2: Standard parameter-shift rule**

**Data:** \( |\psi_0\rangle, \phi, U(x, z) \)

**Result:** \( Q(\phi) \)

**T** ← time (array) ;
\( m \leftarrow 401 ; \)
**for** \( t \) **in** \( T \) **do**

\[
\begin{align*}
x &= 2t \cos(\phi)/m \\
z &= 2t \sin(\phi)/m \\
dx &= U(x + \pi, z) |\psi_0\rangle \\
dz &= U(x, z + \pi) |\psi_0\rangle \\
d\phi &= t [-\sin(\phi) dx + \cos(\phi) dz]
\end{align*}
\]

**get** \( Q(\phi) \) **from** Eq. (31).

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Acknowledgements
We thank Vu Tuan Hai for technical supports.

Author contributions statement
The sole author carried out all the calculations and wrote the manuscript.

Additional information
Accession codes The computational code is available at: https://github.com/echkon/Stochastic-Parameter-shift-rule
Competing interests: The author declares no competing interests.