Generalizable multi-parameter quantum metrology

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Quantum control can be employed in quantum metrology to improve the precision limit for the estimation of unknown parameters. The optimal control, however, typically depends on the actual values of the parameters which then needs to be designed adaptively with the updated estimations of those parameters. Traditional methods, such as gradient ascent pulse engineering (GRAPE), need to be rerun for each new set of parameters encountered, making the optimization costly especially when many parameters are involved. Here we study the generalizability of optimal control, namely optimal controls that can be systematically updated across a range of parameters with minimal cost. In cases where control channels can completely reverse the shift in the Hamiltonian due to change in parameters, we provide an analytical method which efficiently generates optimal controls for any parameter starting from an initial optimal control found either by GRAPE or reinforcement learning. When the control channels are restricted, the analytical scheme is invalid but reinforcement learning still retains a level of generalizability, albeit in a narrower range. Lastly, in cases where the shift in the Hamiltonian is impossible to be decomposed to available control channels, no generalizability is found for either the reinforcement learning or the analytical scheme. We argue that the generalization of reinforcement learning is through a mechanism similar to the analytical scheme. Our results provide insights on when and how the optimal control in multi-parameter quantum metrology can be generalized, thereby facilitating efficient implementation of optimal quantum estimation of multiple parameters, particularly for an ensemble of systems with ranges of parameters.

I. INTRODUCTION

One of the main goals of quantum metrology is to identify the highest possible precision for the estimation of unknown parameters, and find practical ways to approach that limit. There have been extensive studies on the optimization of the probe states and the measurements to achieve better precisions [1–4]. Recently, it has been realized that quantum control during the evolution can be optimized to improve the precision in the estimation of a single parameter [5, 6] or multiple parameters [7, 8]. Optimal quantum control method, such as the gradient ascent pulse engineering (GRAPE), has been employed to obtain the optimal controls [6, 8, 9]. The optimal controls, however, typically depend on the values of the parameters, which need to be adaptively updated with the accumulation of measurement data. Such optimization therefore has to be repeated many times, making it resource-consuming and cumbersome. A method that can systematically update optimal controls across a range of parameters with minimal cost, a characteristic termed as generalizability, is then desirable, particularly for the estimation of multiple parameters as the search space becomes much larger, and performing a brand-new search of optimal controls for each set of parameters could become prohibitively expensive.

Reinforcement Learning (RL) is an alternative method that can be used to estimate multiple parameters. The main idea of RL is to convert an optimization problem into a “game”, while the goals and constraints of the problem are encapsulated as rules in the game. A computer agent, through playing the game in an emulator, obtains rewards depending on its performance. A procedure that maximizes rewards therefore leads to an optimized solution of the desired problem. RL has demonstrated its superior power in playing several types of games [10–12]. It has also been shown to improve solutions to many problems in quantum information science [13], quantum control [14–17], and in particular, quantum metrology [18–20]. In a previous work on the single-parameter quantum estimation, we have shown that RL has an important advantage: the generalizability [18]. An agent trained for one value of the parameter can be straightforwardly generalized to other values of the parameter, producing near-optimal controls. This makes RL efficient for quantum estimation with an ensemble of systems where the values of the parameter may vary within a certain range. This generalizability likely arises from the fact that an RL agent typically under-fits the training data [21–23].

The main goal of this paper is to elucidate how the generalizability is maintained in the situation of multi-parameter quantum estimation. To this purpose, we introduce an analytical method which adjusts the controls (already optimal for certain parameters) to reverse the shift of the Hamiltonian stemming from the change of
the parameters so as to maintain the optimality. This analytical method only applies to the situation in which the controls are “complete”, i.e. there are sufficient control channels to absorb the shift in the Hamiltonian. In this situation, generalization using the analytical method is most effective as only the initial control for a chosen set of parameters needs to be found by RL or GRAPE. When the shift in the Hamiltonian due to change in parameters can only be partially absorbed into available control channels, the analytical method is no longer valid. However, RL still provides generalizable optimal control, albeit for a narrower range of parameters, and we believe that the mechanism for the generalizability afforded by RL is similar to the analytical scheme. Lastly, if the shift in the Hamiltonian cannot be decomposed into available control channels, such as the coupling between two spins considered in this paper, neither RL nor the analytical method provides any generalizability. In this case, one has to rerun either RL or GRAPE for each new set of parameters. Our results provide insights on when and how the optimal control in multi-parameter quantum metrology can be generalized, thereby facilitating efficient implementation of optimal quantum estimation of multiple parameters, particularly for an ensemble of systems with ranges of parameters.

The remainder of the paper is organized as follows. In Sec. II we briefly review the theory on multi-parameter estimation and present the two examples considered in this paper. Sec. III explains the methods used in this work, including GRAPE, RL, and the analytical scheme. In Sec. IV we show detailed results on the generalizability applied to the two examples. We then conclude in Sec. V. Necessary details on the implementation of RL is provided in Appendices.

II. MULTI-PARAMETER QUANTUM ESTIMATION

We consider the time evolution of a quantum state described by the master equation [24],

$$\frac{\partial}{\partial t}\rho(t) = \mathcal{L}[\rho(t)],$$

where $\mathcal{L}[\rho(t)] = -i[H, \rho(t)] + \Gamma(\rho(t))$. $\Gamma(\rho(t))$ describes the effect of noises, and $H$ is the Hamiltonian that can be decomposed as

$$H = H_0(\mathbf{x}) + \sum_{i=1}^{P} u_i(t) H_i,$$

where $H_0(\mathbf{x})$ is the free evolution with $\mathbf{x}$, a vector encapsulating the unknown parameters of interest. The terms $u_i(t) H_i$ represent the control [9], and $P$ is the number of available control channels. We discretize the total evolution time $T$ into $N = T/\Delta t$ equal time slices, and a piece-wise constant pulse sequence generates an evolution as

$$\rho(T) = \prod_{j=0}^{N-1} e^{\Delta t \mathcal{L}_j} \rho(0),$$

where $\mathcal{L}_j$ is the superoperator for the $j$th time slice. The control field is described by the sequence of $u_i(j \Delta t)$ on the interval $[0, T]$.

Given a set of positive-operator valued measurement (POVM) $\{\Pi_y\}$, the covariance matrix of the measurements is lower-bounded by [25]

$$\text{cov}(\hat{x}, \Pi_y) \geq \frac{1}{n} \mathcal{F}^{-1}_{\text{cl}}(\Pi_y) \geq \frac{1}{n} \mathcal{F}^{-1},$$

where $\hat{x}$ is the unbiased estimator of $x$ and $n$ is the number of the repetitions. The first inequality is the classical Cramér-Rao bound, where $\mathcal{F}_{\text{cl}}(\Pi_y)$ is the classical Fisher information matrix which depends on the choice of the measurement,

$$\mathcal{F}_{\text{cl},\alpha\beta} = \sum_{y} \frac{\partial_{x, \alpha} p_{y|x} \partial_{x, \beta} p_{y|x}}{p_{y|x}},$$

where $p_{y|x} = \text{tr}[\rho(t) \Pi_y]$. The second inequality is the quantum Cramér–Rao bound with $\mathcal{F}$ being the quantum Fisher information matrix, which typically can not be attained for the estimation of multiple parameters [25]. In this work, we focus on the classical Cramér–Rao (CR) bound,

$$|\delta \hat{x}|^2 = \text{tr} \text{cov}(\hat{x}) \geq \text{tr} \mathcal{F}_{\text{cl}}^{-1}.$$

$\text{tr} \mathcal{F}_{\text{cl}}^{-1}$ is the key quantity governing the precision of measurements that will be frequently referred to simply as “the CR bound” in the remainder of the paper.

In the following, we discuss the quantum parameter estimation under local controls on each qubit in the multiple-qubit system. The control Hamiltonian for $m$ qubits is

$$H_c(t) = \sum_{i=1}^{m} u^{(i)}(t) \cdot \sigma^{(i)},$$

where $\sigma^{(i)} = (\sigma_x^{(i)}, \sigma_y^{(i)}, \sigma_z^{(i)})$ and $\sigma^{(i)} = \mathbb{I}^{(1)} \otimes \cdots \otimes \mathbb{I}^{(i-1)} \otimes \sigma_a \otimes \mathbb{I}^{(i+1)} \otimes \cdots \otimes \mathbb{I}^{(m)}$. $I$ is the $2 \times 2$ identity matrix and $a = x, y, z$. The total number of control channels is $P = 3m$. To compare with the optimal controls obtained with GRAPE, we will use the same examples studied in the previous work [8].

**Example 1.** The first example involves a two-qubit system where one qubit is in a magnetic field with both the magnitude and direction unknown. The other qubit acts as an ancillary qubit. The Hamiltonian of the first qubit is

$$H_0 = B \cdot \mathbf{\sigma}^{(1)},$$

where $B = (B \sin \vartheta \cos \varphi, B \sin \vartheta \sin \varphi, B \cos \vartheta)$. The parameters to be estimated are $\mathbf{x} = (B, \vartheta, \varphi)$ characterizing
the strength and direction of the magnetic field. The dephasing on the first qubit can be described by the Lindblad form,

$$\Gamma(\rho(t)) = \gamma \left( \sigma_z^{(1)} \rho(t) \sigma_z^{(1)} - \rho(t) \right), \quad (9)$$

where $\gamma$ is the dephasing rate which is set as $\gamma = 0.2$ in our simulation. We use the maximally entangled state, $|00\rangle + |11\rangle)/\sqrt{2}$, as the probe state, and choose the projective measurement on the Bell bases $(|00\rangle \pm |11\rangle)/\sqrt{2}$ and $(|01\rangle \pm |10\rangle)/\sqrt{2}$.

**Example 2.** The second example is a ZZ-coupled two-qubit system. The Hamiltonian of the free evolution is

$$H_0 = \omega_1 \sigma_z^{(1)} + \omega_2 \sigma_z^{(2)} + g \sigma_z^{(1)} \sigma_z^{(2)}, \quad (10)$$

where $\mathbf{x} = (\omega_1, \omega_2, g)$ are the parameters to be estimated. $\omega_1$ and $\omega_2$ are individual magnetic fields along the $z$-direction, while $g$ is the ZZ coupling strength. Both qubits suffer from dephasing dynamics,

$$\Gamma(\rho(t)) = \sum_{i=1,2} \frac{\gamma_i}{2} \left( \sigma_z^{(i)} \rho(t) \sigma_z^{(i)} - \rho(t) \right), \quad (11)$$

where we set the dephasing rates $\gamma_1 = \gamma_2 = 0.1$ in this work. Under unitary dynamics (i.e., without noise), the optimal probe state for this system is $|++\rangle = (|00\rangle + |01\rangle + |10\rangle + |11\rangle)/2$. We thus use $|++\rangle$ as the probe and the local measurements $|++\rangle|++\rangle, |+\rangle-\rangle|+\rangle-\rangle$ and $|--\rangle|--\rangle$ where $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$.

## III. METHODS

### A. Gradient ascent pulse engineering

For the case with only two parameters, Eq. (6) reduces to $|\delta \mathbf{x}|^2 \geq \det F_{\text{cl}1}/\text{tr } F_{\text{cl}1}$. It is possible to derive the gradient of the CR bound with respect to the control field and perform GRAPE to find appropriate optimal controls [8]. However, for the cases with more than two parameters, as the above two examples, taking the gradient of $\text{tr } F_{\text{cl}1}$ is not straightforward. Ref. [8] has introduced another objective function, $f_0(T)$, as

$$f_0(T)^{-1} = \sum_{\alpha} \frac{1}{F_{\text{cl},\alpha}(T)}, \quad (12)$$

which provides a lower bound to $\text{tr } F_{\text{cl}1}$ since $[F_{\text{cl}1}]_{\alpha\alpha} \geq 1/F_{\text{cl},\alpha}$ and $\text{tr } F_{\text{cl}1} \geq \sum_{\alpha} 1/F_{\text{cl},\alpha}$. Practically, the optimal controls are found by optimizing $f_0(T)$, even though it is not necessarily the optimization of the desired CR bound, $\text{tr } F_{\text{cl}1}$. While we largely follows Ref. [8] to repeat the results obtained with GRAPE, we additionally apply the steepest gradient ascent method [26] and the Adam method [27] to update the control field, which are numerically more efficient than the simple updating scheme employed in Ref. [8].

### B. Reinforcement learning

For the piece-wise control in Eq. (3), we can interpret the optimization problem as a Markov decision process in RL. Fig. 1 shows the schematics of RL. The RL procedure is essentially an interaction between an agent and its environment, the latter of which involves a state space $S$, an action space $A$, and a numerical reward $R$ [21]. The behavior of the agent is defined by a policy. In this work, we use the deterministic policy, namely it always maps $s_j \in S$ to a specific action $a_j \in A$ [28]. At each time step $j$, the agent observes the current state $s_j$ and chooses an action $a_j \in A$ according to its policy. The action $a_j$ constitutes the control $u_j^{(j\Delta t)}$ which steers the quantum state according to the dynamics of the environment described by the time evolution Eq. (1), while the agent receives an immediate reward $r_{j+1}$. The agent then observes state $s_{j+1}$ and conducts action $a_{j+1}$ prescribed by the environment. This procedure is iterated until the target time $T$ (or total number of step $N$) is reached, concluding one episode of RL. Each episode is summarized by a trajectory of states, actions, and rewards as $(s_0, a_0, r_1, s_1, \ldots, a_{N-1}, r_N, s_N)$. A replay memory is used to store $(s_j, a_j, r_{j+1}, s_{j+1})$ (termed as a “sample”) at each time step in the iteration. The RL agent is then trained using samples from the replay memory,
which stabilizes the learning process \[10, 29\].

Since the action \(a_j\) influences not only the immediate reward \(r_{j+1}\) but also the future rewards \(r_{k>j+1}\), the immediate reward alone is not an appropriate objective for training the RL agent. To take into account the future rewards, we define the total discounted reward \(R_j = \sum_{k=j}^{N} \alpha_k \cdot r_{k+1}\) with \(\alpha_k \in [0, 1]\) the discount rate \[21\]. In practice, noises must be added to the actions chosen so as to prevent the simulation being trapped in a local minimum \[28, 30\]. Therefore, \(R_j\) can have different values across different episodes, depending on the policy and the dynamics of the environment. We therefore use the expectation value \(E[R_j]\) across all episodes associated to the given deterministic policy and dynamics, \(E[R_j]\), as our objective. Practically, the RL agent maximizes the expected value of the total discounted reward at the initial state, \(E[R_0]\) \[21\].

In this work, we assume that the density matrix, \(\rho(j\Delta t)\), of any quantum state concerned is fully known to the agent \[13, 18, 19\], which may not be true in experiments \[31, 32\]. Our numerical simulation can be viewed as an emulator with regards to the RL procedure. In our numerical simulation, we must guess a value of the parameter \(\delta H\) at each time slice, \(\delta H_{j+1} = \delta H_j + \delta H\). Consequently, the states \(\rho_{j+1}\) can have different values across all episodes associated to the new one, \(\rho_{j+1} = \rho_j + \delta H\), so that it can offer a high precision of estimation at the new parameters. We emphasize that this method can only be used on a known initial control optimized at a specific parameter, with “complete” control channels available to reverse changes in the Hamiltonian.

The Hamiltonian of the new value \(x'\) can be rewritten as

\[ H(x') = H_0(x) + \delta H + \sum_{i=1}^{P} u_i(t)H_i, \]

where \(\delta H = H_0(x') - H_0(x)\) is the change of the Hamiltonian of free evolution. \(H_i(t) = \sum_{j=1}^{P'} u_i(t)H_j\) is the control Hamiltonian on the total of \(P\) channels.

**Lemma 1.** If the states \(\rho_{x'} = \rho_x\) and the partial derivatives \(\partial_{x'}\rho_{x'} = \delta H\rho_{x'}\), then the optimality of the measurement \(\delta u\) on \(\rho_{x'}\) yields \(\delta u_{x'}\). The classical Fisher information matrix is then written as

\[ \text{F}(\rho_{x'}) = \text{tr}\left[ \delta H \text{F}(\rho_x) \right] \]

so that,

\[ \text{F}(\rho_{x'}) = \text{tr}\left[ \delta H \text{F}(\rho_x) \right]. \]

Taking the trace of both sides of Eq. (16) leads to the desired equation. \(\square\)

We are interested in the piecewise square pulses of Eq. (3) on the time interval \([0, T]\). The analytical method that generalizes optimal control to other parameters relies essentially on the following theorem:

**Theorem 1.** If \(\delta H\) can be decomposed into the linear combination \(\delta H = \sum_{i=1}^{P} \delta u_iH_i\), and the optimal control \(\{u_i\}\) is known for the Hamiltonian \(H_0(x)\), the optimal control for the Hamiltonian \(H_0(x')\) is

\[ u_i \to u_i - \delta u_i. \]

**Proof.** When the control field \(\{u_i\}\) changes to \(u_i - \delta u_i\) on each time slice,

\[ H(x') = H_0(x) + \delta H + \sum_{i=1}^{P} (u_i - \delta u_i)H_i = H_0(x) + \sum_{i=1}^{P} u_iH_i = H(x), \]

and the superoperators describing the dynamics with respect to \(x'\) are \(L\rho_{x'}(\delta u) = L\rho_{x'}(\delta u)\). Consequently, the states at each time step are \(\rho_{x'(j\Delta t)} = \rho_{x(j\Delta t)}\) according to

**C. Analytical scheme**

We now introduce the method of adjusting the optimal controls obtained for the parameters \(x\) to the new one, \(x' = x + \delta x\), so that it can offer a high precision of estimation at the new parameters. We emphasize that this method can only be used on a known initial control optimized at a specific parameter, with “complete” control channels available to reverse changes in the Hamiltonian.
the state evolution defined by Eq. (3). We can write down the derivative with respect to the parameters $x'_a$ at the final state in the first-order approximation,

$$\frac{\partial \rho_x(T)}{\partial x'_a} = \sum_{j=0}^{N-1} \sum_{i=j+1}^{N-1} e^{\Delta t L_i(x)} \frac{\partial \Delta t L_j(x')}{\partial x'_a} \rho_x(j \Delta t). \quad (19)$$

The partial derivative in the above equation is simply the derivative over the same superoperator but with respect to the new parameters $x'$. We can define a transformation that maps two partial derivatives to each other as its inverse.

The final state in the first-order approximation, usually has an explicit form and satisfies $\partial \rho_x(T) \partial x'_a = \partial \rho_x(T) \partial x_a$. We can rewrite Eq. (19) and obtain,

$$\frac{\partial \rho_x(T)}{\partial x'_a} = \frac{\partial \rho_x(T)}{\partial x_a} \frac{\partial \rho_x(T)}{\partial x'_a}.$$

(20)

We define $\tilde{R}_{a \beta} = \tilde{C}_{a \beta}^{-1}(x') \tilde{C}_{a \beta}(x)$.

In both (a) and (b) cases, such change in Eq. (17) leads to $\partial \rho_x \partial x(T) = \tilde{R}_{a \beta} \partial \rho_x \partial x(T)$. Regarding the parameters $x$, the control $\{u_i\}_\text{opt}$ is optimal in the sense that $\text{tr} F_{cl}^\dagger(x \{u_i\}_\text{opt}) \leq \text{tr} F_{cl}^\dagger(x \{u_i\})$. Since $F_{cl}^\dagger$ is positive semi-definite, we have $\text{tr} F_{cl}^\dagger(x \{u_i\}_\text{opt}) \leq \text{tr} F_{cl}^\dagger(x \{u_i\})$. Then, Lemma 1 immediately guarantees that the adjusted control field of Eq. (17) is optimal for the parameters $x'$. Note that the theorem relies on the fact that the available control channels must be capable to absorb the changes in the Hamiltonian, requiring “complete” channels of control. When the control is limited, e.g. only along one particular direction, the theorem is no longer applicable.

IV. GENERALIZABILITY

In this section, we shall compare results from different methods for ensembles of systems where the parameters take a range of values. In this case, the controls and estimated values of parameters must be updated adaptively [6]. For the analytical method, we firstly optimize the controls for a chosen set of parameters using RL and GRAPE, and then analytically shift the controls with the new set of the parameters according to Theorem 1. Since the analytical scheme directly modifies the control profile, it provides the most efficient method to generalize an optimal control to other parameters. For RL, an emulator for the new estimated value has to be created. The agent runs in the emulator and designs the quantum control by taking the states of each time step, which has a small computational cost $O(N)$. We shall see that the generalizability of RL is retained for most parameters to be measured. We also consider the situation where the control channels are incomplete so the analytical scheme becomes inapplicable, while the generalizability of the RL agent retains in a smaller range. On the other hand, for the change of the ZZ coupling strength in Example 2, both the analytical scheme and the generalizability of RL fail, so the controls must be optimized by RL or GRAPE individually for each new value.

Example 1. For the analytical method, thanks to Theorem 1, once we have the optimal control $u^{(1)}$ for $B$, we can update the control field as $u^{(1)} - (B' - B)$ when the estimation of the parameter is updated to $B'$. At the same time, the RL policy is learned specifically at $B$, then we generalize the trained policy network to the different magnetic field $B'$. In the simulation, the control fields and the RL agents are optimized at $(B, \vartheta, \varphi) = (1, \pi/4, \pi/4)$.

One of the simplest cases is that $B$ and $B'$ are along the same direction. In Theorem 1, the matrix $\tilde{R}$ consists of the ratios $\tilde{R}_{BB} = 1$, $\tilde{R}_{\vartheta\vartheta} = B'/B$ and $\tilde{R}_{\varphi\varphi} = B'/B$. All other elements are zero. The CR bound at the new value of the parameter is given by

$$\text{tr} F_{cl}^\dagger(B') = \delta \tilde{B}^2 + \left( \frac{B}{B'} \right)^2 (\delta \tilde{\vartheta}^2 + \delta \tilde{\varphi}^2), \quad (23)$$

where $\delta \tilde{B}^2$, $\delta \tilde{\vartheta}^2$ and $\delta \tilde{\varphi}^2$ represent the diagonal terms of $F_{cl}^\dagger(B)$. $\text{tr} F_{cl}^\dagger$ diverges at $B = 0$, but with the increase of $B'$ the value of $\text{tr} F_{cl}^\dagger$ decreases and it is lower bounded by $\delta \tilde{B}^2$.

Fig. 2(a) shows the CR bound at the target time $T$ as a function of $B'$, where $B'$ is allowed to vary between $[B - 2\pi/T, B + 2\pi/T]$, while the direction of the magnetic field is fixed at $(\vartheta, \varphi) = (\pi/4, \pi/4)$. In Fig. 2(a), the dark blue and red solid lines correspond to the analytical scheme using the optimized controls obtained with RL and GRAPE at $B = 1$ respectively (for choice of the target time $T$ along with other details in the implementation of RL, see Appendix C). Results for evaluating the generalization of RL at different $B'$ are shown by blue crosses. In addition, the CR bound obtained by rerunning the GRAPE procedure at selected $B'$ is presented in red squares. Results of the CR bound from the generalization of RL is substantially lower than the case without control in a large neighborhood around $B' = 1$, confirming the generalizability. In fact, for $B' > 1$, RL outperforms GRAPE, even if it is not trained nor opti-
RL, comparing the results found at the training point $B' = B = 1$ (cyan lines) and at a point away from the training point $B' = B + 2\pi/T$ (purple lines). Similarity between the two sets of pulses $u^{(1)}$ is evident from the figure, suggesting that RL achieves generalizability through a mechanism similar to Theorem 1, i.e. the reversal of changes of the free evolution by adjusting available controls. In contrast, controls optimized by GRAPE do not have such similarity as can be seen in Fig. 2(c). A detailed investigation also reveals that RL has imposed strong controls $u^{(2)}_c$ on the ancillary qubit, while GRAPE only exerts minimal controls. This indicates that RL has utilized the full capacity of available controls which contributes to its efficiency.

Fixing the strength $B$, we consider the change in the direction $(\vartheta, \varphi)$. Here, we apply the change of variables transforming the spherical coordinates to Cartesian notations [7]. The Jacobian matrix and $\tilde{R}$ are much more complicated, and the classical Fisher information matrix is not necessarily diagonal for $B'$. Nevertheless, for $B' = B = 1$ and varying $(\vartheta', \varphi')$, the CR bound of $B'$ is given by

$$\text{tr} \mathcal{F}_{cl}^{-1}(B') = C_1\delta \tilde{B}^2 + C_2\delta \tilde{\vartheta}^2 + C_3\delta \tilde{\varphi}^2,$$

with

$$\begin{align*}
C_1 &= \cos^2 \vartheta + \sin^2 \vartheta (\cos^2 \varphi \csc^2 \vartheta' \sin^2 \Delta \varphi), \\
C_2 &= \sin^2 \vartheta + \cos^2 \vartheta (\cos^2 \varphi \csc^2 \vartheta' \sin^2 \Delta \varphi), \\
C_3 &= \sin^2 \vartheta \csc^2 \vartheta' \cos^2 \Delta \varphi + \sin^2 \vartheta \sin^2 \Delta \varphi,
\end{align*}$$

where $\Delta \varphi = \varphi' - \varphi$ is the change in $\varphi$. This expression shows that $\Delta \varphi$ hardly shifts the optimal value of the CR bound, but $\vartheta'$ has notable influences on the results. For example, if $\varphi' = \varphi$ and $\vartheta'$ varies, the CR bound would be

$$\text{tr} \mathcal{F}_{cl}^{-1}(B') = \delta \tilde{B}^2 + \delta \tilde{\vartheta}^2 + \sin(\vartheta') \csc(\vartheta') \delta \tilde{\varphi}^2,$$

and $\mathcal{F}_{cl}^{-1}(B')$ is block-diagonal. The change of parameter $\vartheta'$ can have strong influence on the estimation of $\varphi'$. Specifically, the new lower bound $\delta \tilde{\varphi}^2$ has the smallest value at $\vartheta' = \pi/2$ and diverges at $\vartheta' = 0, \pi$, i.e. the poles $|0\rangle, |1\rangle$ on the Bloch sphere.

In Fig. 3 we show the results from the analytical scheme and the generalization of RL concerning the direction of the magnetic field, i.e. $\vartheta'$ and $\varphi'$ are varied within $[0, \pi]$ and $[0, 2\pi]$, respectively. The strength of the magnetic field is fixed at $B = 1$ and RL is trained at $(\vartheta, \varphi) = (\pi/4, \pi/4)$. Fig. 3(a) shows the pseudo-color plot of the CR bound. In a reasonably large neighborhood around the original training point $(\vartheta, \varphi) = (\pi/4, \pi/4)$, the RL-designed pulse sequences produce similar values of $\text{tr} \mathcal{F}_{cl}^{-1}$ to the analytical method, indicating generalizability. Fig. 3(b) and (c) each presents a cut at fixed $\vartheta'$ or $\varphi'$ as indicated by the dashed lines in the right panel of Fig. 3(a). Fig. 3(b) shows results with $\vartheta' = \pi/4$ and $\varphi'$ varying in $[0, 2\pi]$. For the analytical method, it is clear that results initiated by RL have lower CR bounds.

![Figure 2](image_url)

**FIG. 2.** (a) Generalizability for the strength of the magnetic field in Example 1. For RL, we show $\text{tr} \mathcal{F}_{cl}^{-1}$ at the target time $T = 5$ as a function of $B'$ in $[B - 2\pi/T, B + 2\pi/T]$ where $B = 1$. We use the neural networks that are trained at $(B, \vartheta, \varphi) = (1, \pi/4, \pi/4)$ to generate the pulse sequences for $B'$. The blue crosses shows the results of RL. The red squares represent the results using new pulse sequences optimized by GRAPE. The solid dark blue (red) curve show the analytical results using the pulse sequences found by RL (GRAPE) at $(B, \vartheta, \varphi) = (1, \pi/4, \pi/4)$. The dashed gray curve shows the CR bound without control. (b) Representative pulse profiles obtained with RL. The cyan lines show the results of $B' = B$. The purple lines show the results of $B' = B + 2\pi/T$. (c) Representative pulse profiles obtained with GRAPE. The red lines show the results of $B' = B$. The brown lines show the results of $B' = B + 2\pi/T$. Mimized specifically at those points. Moreover, the analytical scheme and the generalization of RL return similar values of the CR bounds, indicating that controls produced by a trained RL agent away from the training point is near optimal. For $|B'| \lesssim 0.3$, no method offers notable improvement as the optimal solution diverges according to Eq. (23). We note that each of the GRAPE point costs on average $\gtrsim 2$ hrs, meaning that rerunning the optimization in a range of $B'$ would be prohibitively expensive. This demonstrates the effectiveness of RL and the analytical approaches.
proves that the optimal CR bound is functions of \( \vartheta \), \( \varphi \), and \( \omega \) as expected from Eq. (25). When the individual magnetic fields \( \omega_k \) vary, it is straightforward to decompose the change \( \delta H \) into local controls \( \sigma_z^{(k)} \). In the analytical scheme, control fields are adapted as \( u_z^{(k)} \rightarrow u_z^{(k)} - (\omega_k - \omega_z) \). Note that the partial derivative of \( \omega_k \) with respect to \( \omega_k \) is not a function of the parameter itself, i.e. \( \tilde{R} = I_3 \) is a 3 \times 3 identity matrix. Thus, Theorem 1 proves that the optimal CR bound always stays at the same value, \( \tr \mathcal{F}_{\omega}^{(3)}(x') = \tr \mathcal{F}_{\omega}^{(3)}(x) \). For the generalization of RL, the RL agent is initially trained to show a high level of generalizability since the parameter itself, i.e. \( \tilde{R} = I_3 \) is a 3 \times 3 identity matrix. Thus, Theorem 1 proves that the optimal CR bound always stays at the same value, \( \tr \mathcal{F}_{\omega}^{(3)}(x') = \tr \mathcal{F}_{\omega}^{(3)}(x) \). For the generalization of RL, the RL agent is initially trained at \( (B, \theta, \varphi) = (1, \pi/4, \pi/4) \), the location of which is denoted by a blue circle. Two cuts (as seen as blue dashed lines) correspond to results shown in (b) and (c). (b) The CR bound as functions of \( \varphi' \) at fixed \( \vartheta' = 0.25\pi \). (c) The CR bound as functions of \( \vartheta' \) at fixed \( \varphi' = 0.25\pi \).

FIG. 3. Generalizability for the direction of the magnetic field in Example 1. The strength of the magnetic field is fixed as \( B = 1 \). (a) Pseudo-color plots showing the CR bound, \( \tr \mathcal{F}_{\omega}^{(3)} \), at the target time \( T = 5 \) as functions of the parameters \( (\vartheta', \varphi') \) in the plane \([0, \pi] \times [0, 2\pi] \). Note that the color bar has a logarithmic scale. Left: the CR bound using the analytical scheme. Right: the CR bound under controls generated by RL using the policy network trained at \( (B, \theta, \varphi) = (1, \pi/4, \pi/4) \), the location of which is denoted by a blue circle. Two cuts (as seen as blue dashed lines) correspond to results shown in (b) and (c). (b) The CR bound as functions of \( \varphi' \) at fixed \( \vartheta' = 0.25\pi \). (c) The CR bound as functions of \( \vartheta' \) at fixed \( \varphi' = 0.25\pi \).

as compared to the case with no control and GRAPE. This is also true in Fig. 3(c), which shows results with \( \varphi' = \pi/4 \) and varying \( \vartheta' \) in \([0, \pi] \). Overall, quantum controls suppress the divergences that appear periodically in the no-control case at \( \varphi' = 0, \pi \) or \( \vartheta' = \pi/2 \), although the value of CR bounds increase to infinity as \( \vartheta' \) approaches to 0 or \( \pi \), as expected from Eq. (25). Scattered points showing results from GRAPE are found to be comparable to its corresponding analytical results, but we emphasize that here each point is a complete re-run of the full algorithm which is very expensive. On the other hand, RL provides sub-optimal results with a much lower cost on the computational resources.

Example 2. The simplest case for coupling between qubits is the ZZ coupling as in Eq. (10). Again, we introduce a change to the parameters, \( x \rightarrow x' \), so \( \delta H = H_0(x') - H_0(x) = \sum_{k=1}^2 (\omega_k' - \omega_k)\sigma_z^{(k)} + (\varphi' - \varphi)\sigma_z^{(1)}\sigma_z^{(2)} \). When the individual magnetic fields \( \omega_k \) change, it is straightforward to decompose the change \( \delta H \) into local controls \( \sigma_z^{(k)} \). In the analytical scheme, control fields are adapted as \( u_z^{(k)} \rightarrow u_z^{(k)} - (\omega_k' - \omega_k) \). Note that the partial derivative of \( \omega_k \sigma_z^{(k)} \) with respect to \( \omega_k \) is not a function of the parameter itself, i.e. \( \tilde{R} = I_3 \) is a 3 \times 3 identity matrix. Thus, Theorem 1 proves that the optimal CR bound always stays at the same value, \( \tr \mathcal{F}_{\omega}^{(3)}(x') = \tr \mathcal{F}_{\omega}^{(3)}(x) \). For the generalization of RL, the RL agent is initially trained at \( (\omega_1, \omega_2, g) = (1.0, 1.2, 0.1) \). Similar to Example 1, the trained RL agent will then be straightforwardly used on a range of \( \omega_1' \) and \( \omega_2' \).

In Fig. 4, we fix the ZZ coupling strength and show the values of the CR bound with varying individual magnetic fields. To better illustrate the results, we fix one of \( \omega_1' \) and \( \omega_2' \) and vary the other. In Fig. 4(a), \( \omega_1' \) are fixed at 1.0 while \( \omega_2' \) varies, and in Fig. 4(b) we fix \( \omega_2' \) at 1.2 and change \( \omega_1' \). In both cases, the CR bounds obtained by the analytical method stay at constant values as noted above. Within the analytical scheme, initial controls obtained by RL give a slightly lower value of the CR bound. Meanwhile, RL shows a high level of generalizability since the CR bound is orders of magnitudes lower than that of no-control cases and is almost the same as those from the

FIG. 4. Generalizability for the individual magnetic fields in Example 2. The ZZ coupling strength is fixed at \( g = 0.1 \). (a) The CR bound as functions of \( \omega_1' \) at fixed \( \omega_2' = 1.0 \). (b) The CR bound as functions of \( \omega_1' \) at fixed \( \omega_2' = 1.2 \).
analytical method for a wide range of values. We have used GRAPE to optimize new control fields for selective $\omega_k$ and the results are presented by red squares. The fluctuation in the optimized values may arise from the fact that the optimization procedure of GRAPE might fall in a local minimum, and that $f_0(T)$ (Eq. (12)) is different from the desired CR bound as noted in Sec. III A.

Under Example 2, we discuss two representative situations where the analytical method becomes inapplicable, where one must either apply GRAPE at each set of parameters or utilize the generalizability of RL.

In the first situation, we restrict the control channels to $\sigma_x^{(1)}$, $\sigma_x^{(2)}$, $\sigma_y^{(1)}$ and $\sigma_y^{(2)}$, so the shift $\delta H \sim \sigma_z^{(k)}$ brought by the change of $\omega_k$ can no longer be absorbed to local controls. In order to test the generalizability, the RL agent is trained at $(\omega_1, \omega_2, g) = (1.0, 1.2, 0.1)$ with the local controls $\sigma_x^{(1)}$, $\sigma_y^{(1)}$, $\sigma_y^{(2)}$ and $\sigma_y^{(2)}$. We study the magnetic field $\omega_k'$ varying within $[1.0 - \pi/T, 1.0 + \pi/T]$ while $\omega_2' = 1.2$. As shown in Fig. 5(a), the generalizability of RL is weaker, with reasonably low CR bounds seen in a smaller range $0.9 \lesssim \omega_1' \lesssim 1.3$ as a direct result of limited control channels.

In the second situation, the coupling strength $g$ changes, and the analytical scheme no longer holds because the change $\delta H \sim \sigma_z^{(1)} \sigma_z^{(2)}$ cannot be simply decomposed into a combination of local controls, even with all control channels in Eq. (7) available. Fig. 5(b) shows the CR bound under RL-designed controls as a function of $g'$, which varies between $[0.1 - \pi/T, 0.1 + \pi/T]$. The RL agent is trained at $(\omega_1, \omega_2, g) = (1.0, 1.2, 0.1)$. The values of CR bound from RL are much higher than the no-control case, negating the generalizability with respect to the ZZ coupling strength. Smaller values of CR bound are attained by GRAPE, which means that the control fields now must either be optimized for every individual $g'$ using GRAPE or using RL but with the agent re-trained at each individual new $g'$ value. Practically, we note that quantum parameter estimation is not the only technique that can derive from a known (initial) optimal control for a given set of parameters to the optimal control for another set of parameters, with minimal cost. The initial optimal control can be found either by RL or GRAPE. When the controls are “complete”, i.e. the shifts in the Hamiltonian due to change in parameters can be completely absorbed in the available control channels, one may generalize the optimal control using analytical method. On the other hand, when the controls are limited such that these shifts cannot be completely absorbed in the available control channels, such as the case in which the control of a spin system is restricted to certain directions while the evolution of the spins does not have the restriction, the analytical scheme is invalid. However, RL retains a level of generalizability, albeit for a narrower range. Lastly, if it is impossible to decompose the shift in the Hamiltonian into available controls, such as the ZZ-coupling of two spins in Example 2 considered here, neither RL nor the analytical scheme provides any generalizability and one must spend a lot of resources to rerun either RL or GRAPE for each new set of parameters encountered. The analytical scheme provides important insight on when and how the generalizable optimal control of RL may be implemented, as the way RL generalizes controls is found to be similar to the analytical scheme. Our results should facilitate efficient implementation of optimal quantum estimation of multiple parameters, particularly for an ensemble of systems with ranges of parameters.

V. CONCLUSION

In this work, we discussed the generalizability of the multi-parameter quantum estimation schemes in two representative two-qubit systems in presence of dephasing. The generalizability refers to a characteristic of a method that can derive from a known (initial) optimal control for a given set of parameters to the optimal control for another set of parameters, with minimal cost. The initial optimal control can be found either by RL or GRAPE. When the controls are “complete”, i.e. the shifts in the Hamiltonian due to change in parameters can be completely absorbed in the available control channels, one may generalize the optimal control using analytical method. On the other hand, when the controls are limited such that these shifts cannot be completely absorbed in the available control channels, such as the case in which the control of a spin system is restricted to certain directions while the evolution of the spins does not have the restriction, the analytical scheme is invalid. However, RL retains a level of generalizability, albeit for a narrower range. Lastly, if it is impossible to decompose the shift in the Hamiltonian into available controls, such as the ZZ-coupling of two spins in Example 2 considered here, neither RL nor the analytical scheme provides any generalizability and one must spend a lot of resources to rerun either RL or GRAPE for each new set of parameters encountered. The analytical scheme provides important insight on when and how the generalizable optimal control of RL may be implemented, as the way RL generalizes controls is found to be similar to the analytical scheme. Our results should facilitate efficient implementation of optimal quantum estimation of multiple parameters, particularly for an ensemble of systems with ranges of parameters.
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Appendix A: Practical setup of RL

In DDPG, the RL agent consists of a deep-Q network denoted by \( Q^\mu(s, a|\theta^Q) \) and a (deterministic) policy network denoted by \( \mu(s|\theta) \) which are parameterized by \( \theta^Q \) and \( \theta \) respectively. Here, the state-action value function \( Q^\mu(s_j, a_j) = \mathbb{E}[R_j|s_j, a_j] \) describes the expected total discounted reward of state \( s_j \) for taking the action \( a_j \) [21]. The policy network has two hidden layers with 400 and 300 neurons, respectively. The deep-Q network has two hidden layers with 400 and \((300+P)\) neurons, respectively. \( P \) represents the dimension of the action space i.e. the number of control channels. Note that the second hidden layer in deep-Q network concatenates the data from the output of its first hidden layer and the actions from the policy network. For both networks, the input layers take a 32-dimensional real vector corresponding to the fully known \( 4 \times 4 \) density matrix \( \rho(j\Delta t) \).

The \texttt{elu} activation function [34] is used after their hidden layers, and the final output layer of policy network uses \texttt{tanh} [34] to bound the actions.

The DDPG algorithm adapts two sets of neural networks similar to the deep Q-learning: exploring the RL environment with the one set of networks and training the other set (namely the target networks) using the samples in a replay memory [10, 30]. When performing the update to neural networks, we uniformly choose random samples from the replay memory so that the correlation between successive updates is removed, which reduces the variance of learning [21]. The Adam algorithm is used for the target deep-Q and target policy networks with the learning rate \( 10^{-4} \) [34]. Other hyperparameters are identical to the original DDPG paper [30].

In order to prevent the agent from learning undesirable solutions [21], we define the reward function that has non-zero value only at the target time \( T \),

\[
    r_j = \begin{cases} 
    0 & j \neq N, \\
    100 \sum_{n=1}^4 10^{-10^n} \text{tr} \mathcal{F}_c^{-1} & j = N,
    \end{cases} \quad (A1)
\]

where the exponential encourages the agent to reduce \( \text{tr} \mathcal{F}_c^{-1} \).

Appendix B: Training procedure

Training a neural network is usually time consuming, demanding heavy tuning of hyperparameters. In this section, we investigate the performance of RL under different choices of the hyperparameters and exemplify the RL and GRAPE methods regarding their time complexity. The following simulations use the parameters \((B, \vartheta, \phi) = (1, \pi/4, \pi/4)\) for Example 1 and \((\omega_1, \omega_2, g) = (1.0, 1.2, 0.1)\) for Example 2.

Firstly, the controls in our simulation are piece-wise
square pulses where the strengths of controls, \( u_a^{(i)} \), are directly relevant to the performance of RL. The range, \(|u_a^{(i)}| \leq u_m\), significantly affects the efficiency and stability of the RL procedure. In Fig. 6, results show that the range of control has little effect on \( \text{tr} F^{-1}_{cl} \) at target time \( T \) in Example 1, while the range can significantly affect the performance of RL in Example 2. From these results, we set the range as \(|u_a^{(i)}| \leq 3\) in Example 1 and \(|u_a^{(i)}| \leq 5\) in Example 2.

Secondly, we compare the training of RL using 2000, 10000 and 20000 RL episodes, with results shown in Fig. 7. For both Example 1 and Example 2, we have taken \( T = 5 \) and \( \Delta t = 0.1 \) so there are 50 state-action pairs in each RL episode. The size of replay memory is typically chosen as one tenth of the total state-action pairs \([10]\). The results show that in both cases, RL with less than 10000 RL episodes fails to learn a good policy. In order to make the training satisfactory, we use 10000 RL episodes with replay memory size 50000 in Example 1 and use 20000 RL episodes with replay memory size 100000 in Example 2. When \( T \) is larger than 5, longer RL training episodes and larger replay memory should be adapted accordingly.

Thirdly, we discuss the time complexity of different methods as a function of \( N \), the total number of time slices. As shown in Fig. 8, the RL method scales as \( O(N) \). For the GRAPE methods, the slower one \( O(N^2) \) has repeatedly calculated the master equation, but the faster one \( O(N^3) \) uses more computer memory to store the superoperators. In general, RL requires about \( 10^4 \) episodes to train an RL agent but GRAPE needs about \( 10^2 \) iterations to optimize a control field. For \( T = 5 \) and \( \Delta t = 0.1 \) used in this paper, \( N = 50 \) and the total wall-clock time cost for RL and GRAPE to find the optimal control for a given set of parameters is actually comparable.

**Appendix C: Implementation of RL**

In this section, we explain details of the implementation of RL and compare the optimization from RL and GRAPE on both examples shown in Sec. II. While we largely follows Ref. [8] for GRAPE, we additionally apply the steepest gradient ascent method \([26]\) (results shown as GRAPE-GD) and the Adam method \([27]\) (results shown as GRAPE-Adam) to update the control field, which are numerically more efficient than the simple updating scheme. For RL, the state \( s_j \) is a 32-dimensional vector corresponding to real and imaginary parts of elements in the \( 4 \times 4 \) density matrix \( \rho(j\Delta t) \). The action \( a_j \) is a 6-dimensional vector consists of elements in the control fields \( u^{(1)}(j\Delta t) \) and \( u^{(2)}(j\Delta t) \) on both qubits. For \( j < N - 1 \), the immediate rewards are \( r_{j+1} = 0 \), while \( r_N \) is directly related to the CR bound, \( \text{tr} F^{-1}_{cl} \) (detailed form is shown in Appendix A). In the RL procedure, the strength of the control field has substantial impact on the outcome. A range is therefore imposed on the elements of control fields \( u_a^{(i)}(t)\), \((i = 1, 2)\), to avoid instability...
in the learning process. This range is set empirically as $|u_{a}^{(i)}| \leq 3$ for Example 1 and $|u_{a}^{(i)}| \leq 5$ for Example 2 as explained in Appendix B. No other restrictions on the RL procedure is imposed.

In Fig. 9(a), we show the values of the CR bound evolving from $t = 0$ to the target time $t = T$ for Example 1 under quantum control. Overall, the CR bound is highest in the case of no control, indicating a low precision of the estimation. While all three methods produce lower CR bounds at the target time, spikes occur during the evolution using the GRAPE method, especially immediately before the target time. Instead, the precision under RL steadily saturates to the lowest value as the target time is reached. Results from RL is more desirable as in practice the time to implement the measurement may not be accurate [35, 36], and spikes in the CR bounds could result in a rather low precision when the measurement is not exerted precisely at the targeted time.

The time evolution of the CR bound for Example 2 is shown in Fig. 9(b). Again, results from RL steadily reach the lowest value, while results from all other methods are unstable over the course of the evolution. An interesting observation is that the result with no control is comparable to other methods at the target time, which may be due to the local measurement preventing all methods from reaching asymptotically optimal solutions [1, 8, 25, 37].

The CR bound under controls obtained from GRAPE fluctuates over the course of evolution because the control field is only optimized to minimize the bound at the final time. The RL agent, however, is trained to use samples from the replay memory which breaks temporal correlation in each episode. In other words, the RL agent is trained to gradually steer states towards the final state. Therefore, as the system evolves close to the target time, the state is already very close to the final state, which is optimal for the estimation [6, 8, 18]. This leads to less fluctuations in the results as shown in Fig. 9. Therefore, although both RL and GRAPE are capable to find optimal controls at the target time, results from RL have less fluctuations when the target time is approached, implying certain level of robustness against the fluctuations in the time to exert the measurement.

Assuming that the target time is precisely known, we compare different methods on the optimized CR bound as a function of the final time $T$, namely, we allow $T$ to vary, and use the reciprocal of normalized CR bound, $(T \text{ tr } F_{cl}^{-1})^{-1}$, for comparison. Under the unitary dynamics, the Heisenberg scaling can be attained for both examples [7, 8], corresponding to $(T \text{ tr } F_{cl}^{-1})^{-1} = 4T/3$. In presence of noises, $(T \text{ tr } F_{cl}^{-1})^{-1}$ typically increases at the beginning of the evolution and decreases thereafter [8], suggesting that the averaged profits (each time unit) on the precision limit from the time evolution is maximal at a finite $T$ which is the optimal time to perform the measurement.

For Example 1, Fig. 10(a) shows the results of $(T \text{ tr } F_{cl}^{-1})^{-1}$ v.s. $T$. As can be seen from the figure, the maximal value without control is achieved around $T \approx 1.2$, while the largest $(T \text{ tr } F_{cl}^{-1})^{-1}$ obtained by RL occurs around $3 \lesssim T \lesssim 5$, where the effect from control is maximized. As $T$ further increases, the accumulated dephasing effect becomes dominant and the controls may not optimally counteract the noise. For Example 2, Fig. 10(b) shows that without control, $(T \text{ tr } F_{cl}^{-1})^{-1}$ attains the largest value around $T \approx 3$, but under RL the value of $(T \text{ tr } F_{cl}^{-1})^{-1}$ fluctuates very little between $4 \lesssim T \lesssim 6$, and tend to decrease for $T \gtrsim 6$. To ensure consistency, we have fixed $T = 5$ for both examples in the main text. We also present GRAPE results using the same method of Ref. [8]. As shown in Fig. 10, RL and GRAPE methods give comparable results for most values of $T$, with small differences at certain $T$ values.

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