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Optimal convex approximations of qubit states based on l_1-norm of coherence

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Determining the minimal distance between the target state and the convex combination of given states is a fundamental problem in quantum resource theory, offering critical guidance for experimental implementations. In this paper, we embark on an in-depth exploration of the use of a quantum state prepared by the convex combination of given qubit states to optimally approximate the l_1-norm of coherence of the target quantum state, striving to make the prepared state and the target state as similar as possible. Here, we present the analytical solution for the optimal distance for any N given quantum states. We find that the optimal approximation problem for any $N > 4$ quantum states can be transformed into an optimal approximation problem for no more than four quantum states, which not only significantly streamlines the problem but also proves advantageous for laboratories in terms of material conservation. Ultimately, a one-to-one comparison between the analytical and numerical solutions verifies the effectiveness of our approach.

Keywords: quantum information processing, quantum resource theory, quantum coherence, optimal convex approximations

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1. Introduction

With the rapid advancement of quantum information science, quantum resource theory (QRT)[1–4] has emerged as a cornerstone for unraveling quantum phenomena and driving progress in quantum technologies.[5–10] Its core resources, namely, quantum entanglement,[11–20] quantum coherence,[21–32] quantum discord,[33–40] etc. have attracted significant research attention, especially in terms of their quantification and manipulation. This not only deepens our understanding of the essence of quantum mechanics but also brings unprecedented opportunities in fields such as quantum computing, communication, and metrology.

QRT provides a set of efficient methods for quantitatively describing quantum properties, which have three main parts: free states (resource states), free operations, and measures. One of the most common ways to measure quantum properties is to assess the closest distance between a given quantum state and the set of free states. For example, quantum entanglement measures the minimum distance between a given state and the set of separable states.[41–43] Quantum coherence can be understood as the closest distance between the target state and the set of incoherent states (convex combinations of given reference bases).[44,45] Quantum discord can be regarded as the closest distance between a given state and the set of classical states.[46,47]

Therefore, calculating the closest distance between the target quantum state and the set of convex combination states of the given quantum states has become rather important in QRT. We can envision a scenario where, due to unavailable technology or economic reasons, a quantum state urgently needed in the laboratory cannot be obtained. In such a case, preparing a new quantum state through the convex combination of existing quantum states to optimally approximate the target quantum state, and then using it to perform tasks instead of the target state, clearly has a certain experimental value. At this point, new questions arise: what method should be used to quantify the similarity between the target state and the prepared state, and how can one calculate the probability corresponding to the optimal prepared state and the optimal distance? The authors of Refs. [48–50] optimize the target quantum state (channel) by obtaining a given set of states (channels). Subsequently, the given quantum states are gradually extended from the eigenstates of Pauli matrices to the eigenstates of arbitrary unitary matrices,[51,52] as well as to arbitrary complex-valued states;[53] quantum states are extended from pure states to mixed states;[53] the number of given quantum states is extended from $N = 2, 4, 6$ to any $N > 4$;[54] and a triple uncertainty relation based on optimal approximation is also studied.[55–58]

In the field of quantum information processing, quanti-

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fying the distance between quantum states typically relies on geometric measures such as the trace norm and fidelity. However, these approaches often overlook the essential characteristics of quantum resource consumption. For instance, when two quantum states have similar geometric distances, differences in their coherence resources may lead to significantly divergent information-processing efficiencies. In this paper, we further investigate this issue. Quantum states, owing to their rich quantum properties, give rise to computational capabilities far exceeding those of the classical world. Different quantum properties are applied in various quantum information tasks. If we need to utilize the coherence of a certain quantum state for a quantum information task, yet this quantum state is temporarily unavailable, then approximating the coherence of the target quantum state using a convex combination of available quantum states becomes a favorable option. This is the research objective of this paper: preparing a quantum state using a convex combination of available quantum states to make its coherence closest to that of the target quantum state. It is worth emphasizing that this paper employs the l_1-norm as the coherence measure. In contrast, other measures (such as the l_2-norm and fidelity-based coherence measures) do not satisfy strong monotonicity,[23,59] while the trace-norm-based measure only meets the requirements in specific scenarios, such as the qubit case or some special qutrits. The l_1-norm coherence measure, however, not only captures all the excellent properties of coherence measures (e.g., strong monotonicity and contractivity) but also offers an intuitive physical interpretation and efficient computational performance. Finally, based on the given quantum states, we analytically obtain the optimal distance for approximating the coherence of the target quantum state and the corresponding optimal probabilities. In addition, we find that the optimal approximation problem for $N > 4$ given quantum states can be transformed into an optimal approximation problem for no more than four quantum states. A one-to-one comparison between the numerical solutions and the analytical solutions further verifies the effectiveness of our approach. The remainder of this paper is organized as follows. In Section 2, we study all the optimal convex approximations of the target quantum state based on the l_1-norm of coherence. We obtain the complete analytical expressions for $N = 2$, $N = 3$, $N > 4$. The analytical expression for $N = 4$ can be obtained by analogy with the method for $N = 3$. In Section 3, we use several randomly generated examples to test our analytic results. In Section 4, we summarize our research findings.

2. Optimal approximations of qubit states based on the l_1-norm of coherence

2.1. Optimized framework

First, we describe the problem that awaits optimization. Let us assume that the target quantum state ρ, which researchers intend to utilize, is not directly available in the laboratory setting (e.g., due to experimental constraints such as noise, limited resources, or unachievable pure-state preparation). The target state has been identified as the ideal state for quantum information tasks (e.g., quantum computing gates, quantum error correction and fault-tolerant computation, coherent state transmission, and quantum key distribution). The set $S = \{\rho_n, n = 1, 2, \ldots, N\}$ denotes the collection of currently accessible quantum states in the laboratory, where N represents the number of available quantum states (e.g., $N = 2$ for simple qubit pairs in basic entanglement experiments, $N = 10$ for multi-qubit intermediate states in complex quantum algorithms, or $N \gg 1$ for large-scale quantum communication networks). These states ρ_n can be mixed states or pure states, with N quantifying the scale of the experimental resources (e.g., the number of quantum states manipulable in the lab). Our goal is to prepare a quantum state $\chi = \sum_n p_n \rho_n$ to approximate and optimally approach the target quantum state ρ, so that the coherence between the two quantum states ρ and χ is closest. The quantum state obtained through this approximation process is designated as the optimally prepared quantum state $\chi^{\text{opt}} = \sum_n p_n^{\text{opt}} \rho_n$. Correspondingly, the probability associated with this optimally prepared quantum state χ^{opt} is referred to as the optimal probability vector $\boldsymbol{p}^{\text{opt}} = \left(p_1^{\text{opt}}, p_2^{\text{opt}}, \ldots, p_n^{\text{opt}}\right)^{\text{T}}$ with

$$\left\{p_n^{\text{opt}}\right\} = \arg\min_{\{p_n\}} \left| C(\rho) - C\left(\sum_n p_n \rho_n\right) \right|, \tag{1}$$

where $|\cdot|$ represents the absolute value and $C(\cdot)$ represents the coherence measure of the quantum state.[60–65] Moreover, the distance between the optimally prepared quantum state χ and the target quantum state ρ under such circumstances is defined as the optimal distance

$$D^{\text{opt}}(\rho, \chi) = \min_{\{p_n\}} \left| C(\rho) - C(\sum_n p_n \rho_n) \right|. \tag{2}$$

Calculating the optimal distance for the best convex combination of the given N quantum states confirms that quantum resource loss has been minimized and experimental substitutability is optimal. It should be clarified that the essential distinction between coherence measures and traditional state distances (such as the trace norm) lies in the fact that the former quantifies resource amounts rather than geometric distances. Traditional state distances focus on the overall similarity between two quantum states, whereas the coherence distance

proposed herein emphasizes local substitutability in quantum resource consumption tasks. Specifically, in scenarios involving quantum coherence consumption, two quantum states with different forms but equivalent coherence exhibit superior information processing efficiency compared to states with close state distances.

For the sake of convenience, we consider the l_1-norm of coherence to quantify the coherence of quantum states

$$C_{l_1}(\rho)=\sum_{i\neq j}\left|\rho_{ij}\right|. \tag{3}$$

We find that the l_1-norm of coherence has the following useful properties. (C1): $C_{l_1}(\rho)=0$ if and only if quantum state ρ belongs to the incoherent state set $\mathcal{I}$. (C2) Monotonicity: $C_{l_1}(\rho)$ does not increase under incoherent completely positive and trace-preserving (ICPTP) mappings; that is, $C_{l_1}(\rho)\geq C_{l_1}(\Phi_{\mathrm{ICPTP}}(\rho))$. (C3) Strong monotonicity: $C_{l_1}(\rho)$ does not, increase under selective measurements on average; that is, $C_{l_1}(\rho)\geq\sum_i p_i C_{l_1}(\rho_i)$ for all $\{K_i\}$ with $\sum_i K_i^\dagger K_i=\boldsymbol{I}$, $K_i\mathcal{I}K_i^\dagger\in\mathcal{I}$, $p_i=\mathrm{Tr}(K_i\rho K_i^\dagger)$ and $\rho_i=K_i\rho K_i^\dagger/\mathrm{Tr}(K_i\rho K_i^\dagger)$. (C4) Convexity: $C_{l_1}(\rho)$ does not increase under state mixing; that is, $\sum_i p_i C_{l_1}(\rho_i)\geq C(\sum_i p_i\rho_i)$ for any set of states $\{\rho_i\}$ and any $p_i\geq 0$ with $\sum_i p_i=1$.

Next, we consider this problem in the Bloch representation. We define $\boldsymbol{r}=(x,y,z)^{\mathrm{T}}$ as the Bloch vector of the target quantum state ρ with its elements $r_\alpha=\mathrm{Tr}(\rho\sigma_\alpha)$, where σ are Pauli matrices with $\{\alpha=x,y,z\}$. We define $\boldsymbol{r}_n=(x_n,y_n,z_n)^{\mathrm{T}}$ as the Bloch vector of the n-th quantum state ρ_n in the available quantum state set $\{S\}$ with $r_{n\alpha}=\mathrm{Tr}(\rho_n\sigma_\alpha)$.

Our goal is now to construct an optimal quantum state χ through the convex combination of quantum states in the given set $\{S\}$, such that its l_1-norm of coherence is closest to that of the target quantum state ρ. This problem is equivalent to solving the optimization problem

$$\begin{aligned}D^{\mathrm{opt}}(\rho,\chi)&=\min_{\{p_n\}}\left|C_{l_1}(\rho)-C_{l_1}(\sum_n p_n\rho_n)\right|\\&=\min_{\{p_n\}}\left|\sqrt{x^2+y^2}-\sqrt{(\sum_n p_n x_n)^2+(\sum_n p_n y_n)^2}\right|,\end{aligned} \tag{4}$$

with the constraint $p_n\geq 0$ and $\sum_n p_n=1$. We find that the l_1-norm of coherence depends exclusively on the x and y components of the Bloch vector, with no dependency on the z component. This means that two quantum states with different z-direction components but the same x- and y-direction components can be equivalently regarded as the same quantum state in our approximate coherence task. We now further present an optimization method by considering the number of quantum states in the given set $\{S\}$ (ranging from two, three, and gradually to infinity). Based on the following results, we can directly find the analytical optimal probability vector that optimally approximates the l_1-norm of coherence of the target quantum state, as well as the corresponding optimal distance. Before presenting the formal theorem, we first state a lemma to facilitate the subsequent calculations.

Lemma 1 The optimization problem $Q=\min(\sum_n p_n x_n)^2+(\sum_n p_n y_n)^2$ with the constraint $p_n\geq 0$ and $\sum_n p_n=1$ is a global convex optimization problem. It satisfies the three conditions for convex optimization problems. First, the equality constraint $\sum_n p_n-1=0$ is linear; second, the inequality constraint $p_n\geq 0$ is convex; third, the problem Q to be optimized is a convex function, since the Hessian matrix of this function is positive definite, which can be written as

$$H=\frac{\partial^2 Q}{\partial \boldsymbol{p}^2}=2\boldsymbol{X}\boldsymbol{X}^{\mathrm{T}}+2\boldsymbol{Y}\boldsymbol{Y}^{\mathrm{T}}, \tag{5}$$

where $\boldsymbol{X}=(x_1,x_2,\ldots,x_n)^{\mathrm{T}}$ and $\boldsymbol{Y}=(y_1,y_2,\ldots,y_n)^{\mathrm{T}}$ are column vectors containing n elements. Therefore, the local minimum value of the optimization problem is equivalent to the global minimum value. If the unconstrained global optimal point does not meet the constraint conditions, the optimal point is located at the boundary of the constraint conditions. This property helps to simplify the subsequent optimization steps.

2.2. $N=2$

Theorem 1 Consider the number $N=2$ of quantum states in the given set $\{S\}$. We can specify the following regions:

$$\begin{aligned}&①:\alpha_{11}+\alpha_{22}\neq 0,\quad ②:x^2+y^2<\frac{\alpha_{12}^2}{\alpha_{11}+\alpha_{22}},\\&③:x^2+y^2\geq\frac{\alpha_{12}^2}{\alpha_{11}+\alpha_{22}},\quad ④:x^2+y^2\leq x_1^2+y_1^2,\\&⑤:x^2+y^2\leq x_2^2+y_2^2,\end{aligned} \tag{6}$$

$$\begin{aligned}&⑥:\alpha_{11}\geq 0,\quad ⑧:\alpha_{11}<0, x^2+y^2\geq x_1^2+y_1^2,\\&⑦:\alpha_{22}\geq 0,\quad ⑨:\alpha_{22}<0, x^2+y^2\geq x_2^2+y_2^2,\end{aligned} \tag{7}$$

with

$$\begin{aligned}\alpha_{12}&=x_1y_2-x_2y_1,\\\alpha_{11}&=x_1(x_1-x_2)+y_1(y_1-y_2),\\\alpha_{22}&=x_2(x_2-x_1)+y_2(y_2-y_1).\end{aligned} \tag{8}$$

If the Bloch vector of the given quantum state is located in region $\{①\cap②\cap⑥\cap⑦\}$, the optimal distance is

$$D^{\mathrm{opt}}(\rho,\chi)=\sqrt{\frac{\alpha_{12}^2}{\alpha_{11}+\alpha_{22}}}-\sqrt{x^2+y^2}, \tag{9}$$

and the corresponding optimal probability

$$p_1^{\mathrm{opt}}=\frac{\alpha_{22}}{\alpha_{11}+\alpha_{22}},\quad p_2^{\mathrm{opt}}=\frac{\alpha_{11}}{\alpha_{11}+\alpha_{22}}. \tag{10}$$

If the Bloch vector of the given quantum state is located in region $\{①\cap③\cap④\cap⑥\cap(⑦\cup⑨)\}$, the optimal distance $D^{\rm opt}(\rho,\chi)=0$ and the corresponding optimal probability

$$\begin{aligned} p_1^{\rm opt} &= \frac{\alpha_{22}+\sqrt{(\alpha_{11}+\alpha_{22})(x^2+y^2)-\alpha_{12}^2}}{\alpha_{11}+\alpha_{22}}, \\ p_2^{\rm opt} &= 1-p_1^{\rm opt}. \end{aligned} \tag{11}$$

If the Bloch vector of the given quantum state is located in region $\{①\cap③\cap⑤\cap(⑥\cup⑧)\cap⑦\}$, the optimal distance $D^{\rm opt}(\rho,\chi)=0$ and the corresponding optimal probability

$$\begin{aligned} p_1^{\rm opt} &= \frac{\alpha_{22}-\sqrt{(\alpha_{11}+\alpha_{22})(x^2+y^2)-\alpha_{12}^2}}{\alpha_{11}+\alpha_{22}}, \\ p_2^{\rm opt} &= 1-p_1^{\rm opt}. \end{aligned} \tag{12}$$

For the remaining cases, the optimal solution should be taken at the boundary values of the constraint conditions, that is

$$D^{\rm opt}(\rho,\chi)=\min\{D(p_1=0),D(p_2=0)\}. \tag{13}$$

The proof of Theorem 1 is provided in Appendix A.

Next, we consider several groups of quantum states that are easily obtainable in the laboratory, namely the eigenstates of the Pauli matrices. Let $|0\rangle$ and $|1\rangle$, $|2\rangle\equiv\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$ and $|3\rangle\equiv\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)$, and $|4\rangle\equiv\frac{1}{\sqrt{2}}(|0\rangle+\mathrm{i}\,|1\rangle)$ and $|5\rangle\equiv\frac{1}{\sqrt{2}}(|0\rangle-\mathrm{i}\,|1\rangle)$ represent the eigenstates of the Pauli matrices σ_z, σ_x and σ_y, respectively. We consider the following three groups of available states:

$$B_1'=\{|0\rangle,|1\rangle\},\ B_1''=\{|2\rangle,|3\rangle\},\ B_1'''=\{|2\rangle,|4\rangle\}. \tag{14}$$

For the given state set B_1', the l_1-norm of coherence of the prepared state χ is always zero, which conforms to Case 1 in the derivation process of Theorem 1 and is the worst choice in the optimal approximation coherence model.

For the given state set B_1'', the optimal distance is zero, and the corresponding optimal probability

$$p_1^{\rm opt}=\frac{1\pm\sqrt{x^2+y^2}}{2},\ p_2^{\rm opt}=1-p_1^{\rm opt}. \tag{15}$$

In this case, the l_1-norm of coherence of the target quantum state ρ can be fully prepared, indicating that this group of quantum states has optimal selectivity.

For the given state set B_1''', we find that the best approximation effect is related to the properties of the target quantum state ρ. If $x^2+y^2\geq 1/2$, the optimal distance is zero, and the corresponding optimal probability

$$p_1^{\rm opt}=\frac{1\pm\sqrt{2(x^2+y^2)-1}}{2},\ p_2^{\rm opt}=1-p_1^{\rm opt}. \tag{16}$$

If $x^2+y^2<1/2$, the optimal distance

$$D^{\rm opt}(\rho,\chi)=\frac{\sqrt{2}}{2}-\sqrt{x^2+y^2}, \tag{17}$$

and the corresponding optimal probability

$$p_1^{\rm opt}=p_2^{\rm opt}=\frac{1}{2}. \tag{18}$$

The three examples cited here demonstrate the two-way requirements of the optimal coherence approximation problem for both the target quantum state ρ and the given quantum states in set $\{S\}$. We can now start to consider the case $N=3$.

2.3. $N=3$

Theorem 2 Consider the number $N=3$ of quantum states in the given set $\{S\}$. To facilitate the derivation of exact analytical solutions for the optimal quantum state approximation, we define several parameter regions $\{①,②,③,\ldots,㉘\}$ in Eqs. (B1) to (B9), whose specific forms can be found in Appendix B.

If the Bloch vector of the given quantum state is located in region $\{①\cap②\cap③\cap(⑤\cup⑥)\cap(⑦\cup⑧)\}$ or region $\{①\cap②\cap④\cap[⑬\cup⑭\cup(⑮\cap⑰)\cup(⑯\cap⑰)]\cap(⑱\cup⑲)\cap(⑳\cup㉑)\}$, the optimal distance $D^{\rm opt}(\rho,\chi)=0$, and the corresponding optimal probability

$$\begin{aligned} p_1^{\rm opt} &= \Big[-p_2^{\rm opt}(x_{123}+\alpha_{33})+\alpha_{33} \\ &\quad+\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-(p_2^{\rm opt}\tau+\alpha_{13})^2}\Big]/(\alpha_{11}+\alpha_{33}), \\ p_3^{\rm opt} &= 1-p_1^{\rm opt}-p_2^{\rm opt}, \end{aligned} \tag{19}$$

where $p_2^{\rm opt}$ can be any real number between zero and one that meets the above constraints of the region and

$$\begin{aligned} \alpha_{13} &= x_1y_3-x_3y_1, \\ \alpha_{11} &= x_1(x_1-x_3)+y_1(y_1-y_3), \\ \alpha_{33} &= x_3(x_3-x_1)+y_3(y_3-y_1), \\ x_{123} &= x_2(x_1-x_3)+y_2(y_1-y_3). \end{aligned} \tag{20}$$

If the Bloch vector of the given quantum state is located in region $\{①\cap②\cap③\cap(⑨\cup⑩)\cap(⑪\cup⑫)\}$ or region $\{①\cap②\cap④\cap(⑬\cup⑭)\cap(㉒\cup㉓)\cap[㉔\cup㉕\cup(㉖\cap㉘)\cup(㉗\cap㉘)]\}$, the optimal distance $D^{\rm opt}(\rho,\chi)=0$, and the corresponding optimal probability

$$\begin{aligned} p_1^{\rm opt} &= \Big[-p_2^{\rm opt}(x_{123}+\alpha_{33})+\alpha_{33} \\ &\quad-\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-(p_2^{\rm opt}\tau+\alpha_{13})^2}\Big]/(\alpha_{11}+\alpha_{33}), \\ p_3^{\rm opt} &= 1-p_1^{\rm opt}-p_2^{\rm opt}, \end{aligned} \tag{21}$$

where $p_2^{\rm opt}$ can be any real number between zero and one that meets the above constraints of the region.

For the remaining cases, the optimal solution should be taken at the boundary values of the constraint conditions, that is

$$D^{\rm opt}(\rho,\chi)=\min\{D(p_1=0),D(p_2=0),D(p_3=0)\}, \tag{22}$$

which can be solved using Theorem 1. The proof of Theorem 2 is provided in Appendix C.

2.4. $N = 4$

Theorem 3 Consider the number $N = 4$ of quantum states in the given set $\{S\}$. We set the following parameters:

$$\begin{aligned}
\tau_{123} &= x_1(y_2-y_3)+x_2(y_3-y_1)+x_3(y_1-y_2),\\
\tau_{124} &= x_1(y_2-y_4)+x_2(y_4-y_1)+x_4(y_1-y_2),\\
\tau_{234} &= x_2(y_3-y_4)+x_3(y_4-y_2)+x_4(y_2-y_3),\\
\tau_{134} &= x_1(y_3-y_4)+x_3(y_4-y_1)+x_4(y_1-y_3). \qquad (23)
\end{aligned}$$

If the Bloch vector of the given quantum state is located in region $\{\tau_{123}\neq 0,\tau_{124}\neq 0,\tau_{134}\neq 0,\tau_{234}\neq 0\}$, the optimal distance $D^{\rm opt}(\rho,\chi)=0$, and the corresponding optimal probability

$$p_1^{\rm opt\pm}=\frac{-p_2^{\rm opt}\beta_{124}-p_3^{\rm opt}\beta_{134}+\alpha_{44}\pm\sqrt{\Delta}}{\alpha_{11}+\alpha_{44}}, \qquad (24)$$

with

$$\begin{aligned}
&\alpha_{14}=x_1y_3-x_3y_1,\\
&\alpha_{11}=x_1(x_1-x_3)+y_1(y_1-y_3),\\
&\alpha_{44}=x_3(x_3-x_1)+y_3(y_3-y_1), \qquad (25)\\
&\beta_{124}=(x_1-x_4)(x_2-x_4)+(y_1-y_4)(y_2-y_4),\\
&\beta_{134}=(x_1-x_4)(x_3-x_4)+(y_1-y_4)(y_3-y_4),\\
&\Delta=(x^2+y^2)(\alpha_{11}+\alpha_{44})-(p_2\tau_{124}+p_3\tau_{134}+\alpha_{14})^2. \qquad (26)
\end{aligned}$$

The necessary condition for the optimal distance $D^{\rm opt}(\rho,\chi)=0$ is that for the given quantum state, there exist $\{p_2^{\rm opt},p_3^{\rm opt}\in[0,1]\}$ such that $\Delta\geq 0$ and $p_1^{opt\pm}\in[0,1]$ are true.

For the remaining cases, the optimal solution should be taken at the boundary values of the constraint conditions, that is

$$\begin{aligned}
&D^{\rm opt}(\rho,\chi)\\
&=\min\{D(p_1=0),D(p_2=0),D(p_3=0),D(p_4=0)\}, \qquad (27)
\end{aligned}$$

which can be solved using Theorem 2.

Proof Consider the number $N=4$ of quantum states in the given set $\{S\}$. For $N=4$, equation (4) can be specifically rewritten as

$$\begin{aligned}
&D^{\rm opt}(\rho,\chi)\\
&=\min_{\{p_1,p_2,p_3,p_4\}}\left|\sqrt{x^2+y^2}-\sqrt{Q(p_1,p_2,p_3,p_4)}\right| \qquad (28)
\end{aligned}$$

with $Q(p_1,p_2,p_3,p_4)=(p_1x_1+p_2x_2+p_3x_3+p_4x_4)^2+(p_1y_1+p_2y_2+p_3y_3+p_4y_4)^2$. For convenience, we set

$$\begin{aligned}
\tau_{123} &= x_1(y_2-y_3)+x_2(y_3-y_1)+x_3(y_1-y_2),\\
\tau_{124} &= x_1(y_2-y_4)+x_2(y_4-y_1)+x_4(y_1-y_2),\\
\tau_{234} &= x_2(y_3-y_4)+x_3(y_4-y_2)+x_4(y_2-y_3),\\
\tau_{134} &= x_1(y_3-y_4)+x_3(y_4-y_1)+x_4(y_1-y_3). \qquad (29)
\end{aligned}$$

Case 1 $\tau_{123}=0$ or $\tau_{124}=0$ or $\tau_{134}=0$ or $\tau_{234}=0$.

The condition $\tau_{123}=0$ implies that three points $\{(x_1,y_1),(x_2,y_2),(x_3,y_3)\}$ in the Euclidean space are collinear. At this time, one of the points can be expressed as the convex combination of the other two points, and its effect can be neglected. Therefore, Case 1 means that among the four points, there are always three points that are collinear. Therefore, the optimal approximation effect of the four quantum states can be replaced by three of them, and the optimal value is located at the boundary conditions of the constraint condition as follows:

$$\begin{aligned}
&D^{\rm opt}(\rho,\chi)\\
&=\min\{D(p_1=0),D(p_2=0),D(p_3=0),D(p_4=0)\}. \qquad (30)
\end{aligned}$$

Case 2 $\tau_{123}\neq 0$, $\tau_{124}\neq 0$, $\tau_{134}\neq 0$, $\tau_{234}\neq 0$.

Considering that the function $Q(p_1,p_2,p_3,p_4)=(p_1x_1+p_2x_2+p_3x_3+p_4x_4)^2+(p_1y_1+p_2y_2+p_3y_3+p_4y_4)^2$ is a convex function, its minimum value without the constraint that $p_n\in[0,1]$ is located at

$$\begin{aligned}
p_1 &= \frac{p_3\tau_{234}+x_2y_4-x_4y_2}{\tau_{124}},\\
p_2 &= \frac{-p_3\tau_{134}+x_1y_4-x_4y_1}{\tau_{124}},\\
p_4 &= 1-p_1-p_2-p_3, \qquad (31)
\end{aligned}$$

where p_3 can take any value, and

$$Q_{\min}(p_1,p_2,p_3,p_4)=0. \qquad (32)$$

This means that the function $Q_1=x^2+y^2$ and the function Q always have intersection points, even in the absence of the constraint conditions $p_n\in[0,1]$. Next, we will start to solve the analytical solutions of the intersection points. In other words, we will consider the situation where the optimal distance is zero, that is to say,

$$\begin{aligned}
&F(p_1,p_2,p_3,p_4)\\
&=Q(p_1,p_2,p_3,p_4)-(x^2+y^2)\\
&=p_1^2[(x_1-x_4)^2+(y_1-y_4)^2]+2p_1[p_2(x_1-x_4)(x_2-x_4)\\
&\quad+p_2(y_1-y_4)(y_2-y_4)+p_3(x_1-x_4)(x_3-x_4)\\
&\quad+p_3(y_1-y_4)(y_3-y_4)+x_4(x_1-x_4)+y_4(y_1-y_4)]\\
&\quad+[p_2(x_2-x_4)+p_3(x_3-x_4)+x_4]^2\\
&\quad+[p_2(y_2-y_4)+p_3(y_3-y_4)+y_4]^2-(x^2+y^2)\\
&=0.
\end{aligned}$$

The solution of the above equation is

$$p_1^{\pm}=\frac{-p_2\beta_{124}-p_3\beta_{134}+\alpha_{44}\pm\sqrt{\Delta}}{\alpha_{11}+\alpha_{44}} \qquad (33)$$

with

$$\begin{aligned}
&\alpha_{14} = x_1y_3 - x_3y_1,\\
&\alpha_{11} = x_1(x_1-x_3) + y_1(y_1-y_3),\\
&\alpha_{44} = x_3(x_3-x_1) + y_3(y_3-y_1),\\
&\beta_{124} = (x_1-x_4)(x_2-x_4) + (y_1-y_4)(y_2-y_4),\\
&\beta_{134} = (x_1-x_4)(x_3-x_4) + (y_1-y_4)(y_3-y_4),
\end{aligned} \tag{34}$$

$$\Delta = (x^2+y^2)(\alpha_{11}+\alpha_{44}) - (p_2\tau_{124} + p_3\tau_{134} + \alpha_{14})^2. \tag{35}$$

Now our focus is whether $\{p_2, p_3 \in [0,1]\}$ exist for the Bloch vector parameters of the given quantum state, such that $\Delta \geq 0$ and $p_1^{\pm} \in [0,1]$. That is to say, we calculate the necessary conditions when $\Delta \geq 0$ and $p_1^{\pm} \in [0,1]$. The calculation process is similar to Eqs. (C9)–(C130) in Appendix C when $N = 3$. We do not elaborate on it here. For the given quantum state, if there are appropriate $\{p_2, p_3 \in [0,1]\}$, then the optimal distance is zero, and the optimal probability is shown as in Eq. (33). If there is no such $\{p_2, p_3 \in [0,1]\}$, then the optimal value is located at the boundary conditions in Eq. (30). The proof is complete.

2.5. $N > 4$

Theorem 4 Consider the number $N > 4$ of quantum states in the given set $\{S\}$. The optimal distance is determined by

$$\begin{aligned}
&D^{\rm opt}(\rho, \chi_{1,2,\ldots,N})\\
&= \min_{i_1<i_2<\cdots<i_N} D^{\rm opt}(\rho, \chi_{i_1,i_2,i_3,i_4}),\ \ i_1,i_2,i_3,i_4 = 1,2,3,4.
\end{aligned} \tag{36}$$

Proof Consider the number $N > 4$ of quantum states in the given set $\{S\}$. For $N > 4$, Eq. (4) can be specifically rewritten as

$$\begin{aligned}
&D^{\rm opt}(\rho, \chi)\\
&= \min_{\{p_n\}} \left| \sqrt{x^2+y^2} - \sqrt{Q(p_n)} \right|,\ \ \{n = 1,2,\cdots,N\},
\end{aligned} \tag{37}$$

with $Q(p_n) = \sum_n^N (p_n x_n)^2 + \sum_n^N (p_n y_n)^2$. We assume that $\{p_n^{\rm opt}\}$ is the optimal probability corresponding to the optimal distance. At this time, the optimally prepared quantum state is $\chi^{\rm opt} = \sum_n^N p_n^{\rm opt}\rho_n$, and its corresponding Bloch vector is

$$\boldsymbol{r}^{\rm opt} = \sum_n^N p_n^{\rm opt}\boldsymbol{r}_n. \tag{38}$$

Carathéodory's theorem[66,67] states that if a point x of R^d lies in the convex hull of a set $\{\Xi\}$, there is a subset $\{\tilde{\Xi}\}$ of $\{\Xi\}$ consisting of $d+1$ or fewer points such that x lies in the convex hull of $\{\tilde{\Xi}\}$. In this paper, if $\boldsymbol{r}^{\rm opt}$ belongs to the convex combination set $\{S\}$ of n Bloch vectors, then it must belong to the subset $\{\tilde{S}\}$ which is composed of the convex combinations of no more than four Bloch vectors in the set $\{\tilde{S}\}$, which can be expressed as

$$\boldsymbol{r}^{\rm opt} = \sum_n^4 q_n^{\rm opt}\boldsymbol{r}_n \tag{39}$$

with $\sum_n^4 q_n^{\rm opt} = 1$ and $q_n^{\rm opt} \geq 0$. Therefore, when $N > 4$, the optimal quantum state prepared by the optimal convex combination of N quantum states can be achieved through the convex combination of no more than four of those quantum states, which can be expressed as

$$\chi^{\rm opt} = \sum_n^4 q_n^{\rm opt}\rho_n. \tag{40}$$

That is to say, for the given N quantum states, we directly consider the optimal convex approximation of all combinations of four quantum states in the set $\{S\}$, and its minimum value is equal to the optimal distance of the N quantum states we want, which can be expressed as

$$\begin{aligned}
&D^{\rm opt}(\rho, \chi_{1,2,\ldots,N})\\
&= \min_{i_1<i_2<\cdots<i_N} D^{\rm opt}(\rho, \chi_{i_1,i_2,i_3,i_4}),\ \ i_1,i_2,i_3,i_4 = 1,2,3,4.
\end{aligned} \tag{41}$$

The proof is complete.

3. Examples

Next, we further prove the validity of our results through a comparison between the analytical solutions and the numerical solutions in specific cases. The target qubit state ρ can be parameterized as

$$\rho = \begin{pmatrix} 1-a & k\sqrt{a(1-a)}\,e^{-i\Phi} \\ k\sqrt{a(1-a)}\,e^{i\Phi} & a \end{pmatrix} \tag{42}$$

with $k, a \in [0,1]$ and $\Phi \in [0, 2\pi]$ denoting the phase, and its corresponding Bloch vector is

$$\begin{aligned}
&x = 2k\sqrt{a(1-a)}\cos\Phi,\ \ y = 2k\sqrt{a(1-a)}\sin\Phi,\\
&z = 1-2a.
\end{aligned} \tag{43}$$

The quantum states are randomly generated by MATLAB. Here, we present the Bloch vector representation of the quantum states, which satisfies $x_n^2 + y_x^2 + z_n^2 \leq 1$, where the equal sign indicates a pure state.

(i) $N = 2$. $S = \{\rho_1, \rho_2\}$ with

$$\begin{aligned}
\boldsymbol{r}_1 &= (-0.48085, 0.00375, 0.59163)^{\rm T},\\
\boldsymbol{r}_2 &= (0.03153, 0.1027, 0.060348)^{\rm T}.
\end{aligned} \tag{44}$$

In Fig. 1(a), the target qubit state ρ is given by the randomly generated phase $\Phi = 0.87809\pi$. The optimal distance denoted by $D(\rho, \chi)$ versus $a \in [0,1]$ is plotted in Fig. 1(a), where the dotted blue, solid red, dashed green, and dashed–dotted magenta lines correspond to the increasing order of variables $\{k = 0, 0.3, 0.6, 0.9\}$, respectively. Similarly, the optimal distance $D(\rho, \chi)$ versus $k \in [0,1]$ is plotted in Fig. 1(b), with the

fixed parameter $a = 0.79005$ and the dotted blue, solid red, dashed green, and dash-dot magenta lines correspond to the increasing order of variables $\{\Phi = 0, 0.5\pi, \pi, 1.5\pi\}$. It can be seen that our analytical solution and the numerical solution are almost identical, thus verifying the validity of our solution. In Fig. 1(b), the four curves coincide because for different values of $\{\Phi = 0, 0.5\pi, \pi, 1.5\pi\}$, the absolute values of the off-diagonal elements of the matrix are the same, and the corresponding l_1-norm of coherence is the same. This shows that the phase has no impact on the l_1-norm of coherence, and this property is also reflected in Fig. 1(b).

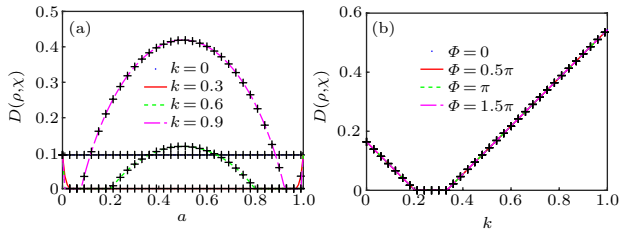


Fig. 1. The optimal distance $D(\rho,\chi)$ is plotted versus various parameters a in (a) and various parameters k in (b). The solid line corresponds to the analytical expression we provided, while the "+" marks represent the numerical solution. The numerical solutions are obtained via an exhaustive search: we sample p_1 at intervals of 0.001 (i.e., $p_1 = 0:0.001:1$) and set $p_2 = 1 - p_1$ to calculate the distance corresponding to each group of probabilities and find the optimal value among them. Here, the step size is $\Upsilon = 0.001$.

(ii) $N = 3$. $S = \{\rho_1, \rho_2, \rho_3\}$ with

$$\begin{aligned} \boldsymbol{r}_1 &= (-0.12919, -0.095161, 0.076729)^{\mathrm{T}}, \\ \boldsymbol{r}_2 &= (-0.014732, -0.57121, 0.32737)^{\mathrm{T}}, \\ \boldsymbol{r}_3 &= (0.092076, -0.072787, 0.17789)^{\mathrm{T}}. \end{aligned} \tag{45}$$

In Fig. 2(a), the target qubit state ρ is given by the randomly generated phase $\Phi = 0.1129\pi$. The optimal distance denoted by $D(\rho,\chi)$ versus $k \in [0,1]$ is plotted in Fig. 2(a), where the dotted blue, solid red, dashed green, and dashed–dotted magenta lines correspond to the increasing order of variables $\{a = 0.2, 0.4, 0.6, 0.8\}$, respectively. It can be seen in Fig. 2(a) that the analytical solution we have provided and the numerical solution are almost identical. Interestingly, the two curves with $a = 0.2$ and $a = 0.8$ completely coincide in the figure, and the two curves with $a = 0.4$ and $a = 0.6$ also completely coincide. This is because the qubit state has l_1-norm of coherence "a" symmetry; that is, the optimal distance remains unchanged under the state transformation $\rho(a,k,\Phi) \to \rho(1-a,k,\Phi)$. Figure 2(b) depicts a comparison between numerical solutions of different precisions and the analytical solution. It can be seen that the analytical solution is always superior to the numerical solutions, and as the precision continuously improves, the numerical solutions get closer and closer to the analytical solution. This clearly demonstrates the importance of the analytical solution, which has a high precision that the numerical solutions cannot match.

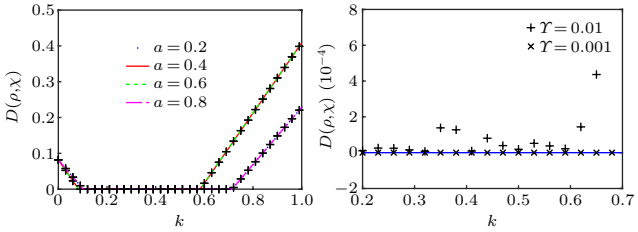


Fig. 2. The optimal distance $D(\rho,\chi)$ is plotted versus various parameters $k \in [0,1]$ in panel (a) and various parameters $k \in [0.2, 0.7]$ in (b). The solid line corresponds to the analytical expression we provided, while the "+" mark represents the numerical solution. The numerical solutions come from the exhaustive method; that is to say, we substitute $p_1 = 0:0.001:1$, $p_2 = 0:0.001:1 - p_1$ and $p_3 = 1 - p_1 - p_2$ to calculate the distance corresponding to each group of probabilities and find the optimal value among them. Here, the step size is $\Upsilon = 0.001$. In panel (b), the solid blue line represents the analytical solution we provided. Different numerical solutions are obtained at different calculation precisions (i.e., different step sizes Υ). Among them, the "+" mark represents a step size of $\Upsilon = 0.01$, and the "x" mark represents a step size of $\Upsilon = 0.001$.

(iii) $N = 8$. $S = \{\rho_1, \rho_2, \rho_3, \rho_4, \rho_5, \rho_6, \rho_7, \rho_8\}$ with

$$\begin{aligned} \boldsymbol{r}_1 &= (0.5955, 0.59374, 0.18064)^{\mathrm{T}}, \\ \boldsymbol{r}_2 &= (-0.10714, 0.14407, 0.52989)^{\mathrm{T}}, \\ \boldsymbol{r}_3 &= (0.56938, 0.28935, -0.02096)^{\mathrm{T}}, \\ \boldsymbol{r}_4 &= (0.76619, -0.59547, -0.20682)^{\mathrm{T}}, \\ \boldsymbol{r}_5 &= (-0.21963, 0.3573, 0.90271)^{\mathrm{T}}, \\ \boldsymbol{r}_6 &= (0.15121, -0.38657, -0.45797)^{\mathrm{T}}, \\ \boldsymbol{r}_7 &= (0.084295, 0.57997, 0.30897)^{\mathrm{T}}, \\ \boldsymbol{r}_8 &= (0.024164, -0.24887, 0.47885)^{\mathrm{T}}. \end{aligned} \tag{46, 47}$$

The Bloch vector of the target quantum state ρ can be represented as

$$\boldsymbol{r} = (0.29086, 0.056474, 0.18361)^{\mathrm{T}}. \tag{48}$$

We find that in this case, the coherence of the target quantum state ρ can be perfectly prepared by the given quantum state set S, i.e., there exists an optimal probability vector

$$\begin{aligned} \boldsymbol{p}^{\mathrm{opt}} = (&0.19883, 0.16658, 0.16136, 0.11887, \\ &0.066964, 0.11764, 0.0027911, 0.16697)^{\mathrm{T}} \end{aligned} \tag{49}$$

such that

$$\boldsymbol{r} = \sum_n^8 p_n^{\mathrm{opt}} \boldsymbol{r}_n. \tag{50}$$

According to Carathéodory's theorem, the optimal quantum state can be prepared by fewer quantum states, that is

$$\begin{aligned} \boldsymbol{r} &= \sum_n^8 p_n^{\mathrm{opt}} \boldsymbol{r}_n \\ &= 0.20417\boldsymbol{r}_1 + 0.15845\boldsymbol{r}_2 + 0.16286\boldsymbol{r}_3 + 0.1109\boldsymbol{r}_4 \\ &\quad + 0.063115\boldsymbol{r}_5 + 0.1193\boldsymbol{r}_6 + 0.18121\boldsymbol{r}_8 \\ &= 0.27072\boldsymbol{r}_1 + 0.029632\boldsymbol{r}_2 + 0.16422\boldsymbol{r}_3 + 0.012652\boldsymbol{r}_4 \\ &\quad + 0.13372\boldsymbol{r}_6 + 0.38906\boldsymbol{r}_8 \end{aligned}$$

$$
\begin{aligned}
&= 0.27916\boldsymbol{r}_1 + 0.001416\boldsymbol{r}_2 + 0.16469\boldsymbol{r}_3 + 0.13851\boldsymbol{r}_6 \\
&\quad + 0.41624\boldsymbol{r}_8 \\
&= 0.10711\boldsymbol{r}_2 + 0.50264\boldsymbol{r}_3 + 0.052823\boldsymbol{r}_6 \\
&\quad + 0.33743\boldsymbol{r}_8. \qquad (51)
\end{aligned}
$$

That is to say, only four quantum states are required at most to achieve the same optimal approximation effect as eight quantum states, which is conducive to the precise control of quantum states in experimental manipulation.

4. Discussion and conclusions

Overall, we aimed to construct a quantum state distance framework based on coherence measures. By quantifying the loss of coherence resources based on the l_1-norm of coherence in the optimal state approximation process, we have bridged the theoretical gap of traditional geometric measures in resource-consumption scenarios. In addition, we have studied the optimal approximation problem of the convex combination of the target quantum state and the given quantum states based on the l_1-norm of coherence, making the coherence between the target state and the prepared state as close as possible, thus laying a foundation for experimental implementation. We impose no restrictions on the given quantum states, which can be either pure states or mixed states, or even any quantum states in the complex domain. In this regard, our approach has strong practical significance. In this paper, we provide the analytical expressions for the optimal distance and the corresponding optimal probability for the quantum state numbers $N = 2$, $N = 3$, $N = 4$, and $N > 4$. Moreover, we gradually expanded the number of quantum states and found that the optimal convex approximation problem of any number of quantum states such that $N > 4$ can be transformed into the optimal convex approximation problem of no more than four quantum states. This greatly simplifies the calculation process and has guiding significance for laboratory operations. Finally, we would like to emphasize that the analytical solutions derived for the optimal quantum state approximation exhibit inherently higher precision than numerical methods and can help to better understand the physical phenomena therein.

Furthermore, our approach is extensible. In this paper, we mainly focused on the qubit system. It would be interesting to further generalize these results to higher-dimensional systems or use other more appropriate coherence measures, such as those based on skew information, relative entropy, etc. It is also possible to consider applying this method to specific experimental operations, comparing the actual usage differences between the target state and the optimal prepared state, and further enhancing its research significance.

Appendix A: Proof of Theorem 1

For $N = 2$, equation (4) can be specifically rewritten as follows:

$$
\begin{aligned}
D^{\mathrm{opt}}(\rho,\chi) = \min_{\{p_1,p_2\}} \Big| & \sqrt{x^2+y^2} \\
& - \sqrt{(p_1x_1+p_2x_2)^2+(p_1y_1+p_2y_2)^2} \Big|.
\end{aligned}
$$

For convenience, we set

$$
\begin{aligned}
\alpha_{12} &= x_1y_2 - x_2y_1, \\
\alpha_{11} &= x_1(x_1-x_2) + y_1(y_1-y_2), \\
\alpha_{22} &= x_2(x_2-x_1) + y_2(y_2-y_1). \qquad (A1)
\end{aligned}
$$

Case 1 $\alpha_{11}+\alpha_{22}=0$.

In this case, we have $x_1 = x_2$ and $y_1 = y_2$. Therefore, the convex combination of these two quantum states with any probabilities is equal to a constant value. For any $p_n \in [0,1]$, the optimal distance

$$
D^{\mathrm{opt}}(\rho,\chi) = \left| \sqrt{x^2+y^2} - \sqrt{x_1^2+y_1^2} \right|. \qquad (A2)
$$

Case 2 $\alpha_{11}+\alpha_{22} \neq 0$.

Considering that the function $Q(p_1,p_2) = (p_1x_1 + p_2x_2)^2 + (p_1y_1+p_2y_2)^2$ is a convex function, its minimum value without the constraint that $p_n \in [0,1]$ is located at

$$
p_1 = \frac{\alpha_{22}}{\alpha_{11}+\alpha_{22}}, \quad p_2 = \frac{\alpha_{11}}{\alpha_{11}+\alpha_{22}}, \qquad (A3)
$$

$$
Q_{\min}(p_1,p_2) = \frac{\alpha_{12}^2}{\alpha_{11}+\alpha_{22}}. \qquad (A4)
$$

We first consider the situation where the minimum value of the function Q is greater than the square of the l_1-norm of coherence of the target state ρ. In this case, it is impossible to fully prepare the same coherence as that of the target quantum state ρ.

Case 2.1 $x^2+y^2 < \frac{\alpha_{12}^2}{\alpha_{11}+\alpha_{22}}$.

Case 2.1.1 $\alpha_{11} \geq 0,\ \alpha_{22} \geq 0$.

Under these constraints, the optimal distance is

$$
D^{\mathrm{opt}}(\rho,\chi) = \sqrt{\frac{\alpha_{12}^2}{\alpha_{11}+\alpha_{22}}} - \sqrt{x^2+y^2}, \qquad (A5)
$$

and the corresponding optimal probability is given by Eq. (A3).

Case 2.1.2 $\alpha_{11} < 0$.

Under this constraint, the optimal distance is

$$
D^{\mathrm{opt}}(\rho,\chi) = \sqrt{x_1^2+y_1^2} - \sqrt{x^2+y^2}, \qquad (A6)
$$

and the corresponding optimal probability

$$
p_1^{\mathrm{opt}} = 1, \quad p_2^{\mathrm{opt}} = 0, \qquad (A7)
$$

which is located at the boundary of the constraint conditions.

Case 2.1.3 $\alpha_{22} < 0$.

Under this constraint, the optimal distance is

$$D^{\rm opt}(\rho,\chi)=\sqrt{x_2^2+y_2^2}-\sqrt{x^2+y^2}, \tag{A8}$$

and the corresponding optimal probability

$$p_1^{\rm opt}=0,\ \ p_2^{\rm opt}=1, \tag{A9}$$

which is located at the boundary of the constraint conditions.

Next, we consider the situation where the minimum value of the function Q is greater than or equal to the square of the l_1-norm of coherence of the target state ρ. In this case, it is possible to fully prepare the same coherence as that of the target quantum state ρ, which requires that the minimum value of the function Q lies within the scope of the constraint conditions. If the minimum value is not within the scope of the constraint conditions, according to the properties of convex optimization problems, we can look for the optimal value at the boundary of the function. The specific situations are as follows.

Case 2.2 $x^2+y^2\geq\frac{\alpha_{12}^2}{\alpha_{11}+\alpha_{22}}$.

Under this constraint, we consider the situation where the optimal distance is zero, that is to say,

$$\begin{aligned}F(p_1,p_2)&=(p_1x_1+p_2x_2)^2+(p_1y_1+p_2y_2)^2-(x^2+y^2)\\&=p_1^2[(x_1-x_2)^2+(y_1-y_2)^2]+x_2^2+y_2^2\\&\quad-(x^2+y^2)+2p[x_2(x_1-x_2)+y_2(y_1-y_2)]\\&=p_1^2(\alpha_{11}+\alpha_{22})-2p_1\alpha_{22}+x_2^2+y_2^2-(x^2+y^2)\\&=0.\end{aligned} \tag{A10}$$

The solution to the above equation is

$$p_1^{\pm}=\frac{\alpha_{22}\pm\sqrt{(\alpha_{11}+\alpha_{22})(x^2+y^2)-\alpha_{12}^2}}{\alpha_{11}+\alpha_{22}}. \tag{A11}$$

Case 2.2.1 $0\leq p_1^+\leq 1$.

Among them, the equivalent condition for $p_1^+\leq 1$ is

$$\alpha_{11}\geq 0,\ \ x^2+y^2\leq x_1^2+y_1^2. \tag{A12}$$

The equivalent condition for $p_1^+\geq 0$ is

$$\alpha_{22}\geq 0, \tag{A13}$$

or

$$\alpha_{22}<0,\ \ x^2+y^2\geq x_2^2+y_2^2. \tag{A14}$$

Case 2.2.2 $0\leq p_1^-\leq 1$.

Similarly, the equivalent condition for $p_1^-\leq 1$ is

$$\alpha_{11}\geq 0, \tag{A15}$$

or

$$\alpha_{11}<0,\ \ x^2+y^2\geq x_1^2+y_1^2. \tag{A16}$$

The equivalent condition for $p_1^-\geq 0$ is

$$\alpha_{22}\geq 0,\ \ x^2+y^2\leq x_2^2+y_2^2. \tag{A17}$$

When the given quantum states satisfy the condition described by the Eqs. {(A12)∩[(A13)∪(A14)]} or the Eqs. {[(A15)∪(A16)]∩(A17)}, the optimal distance

$$D^{\rm opt}(\rho,\chi)=0, \tag{A18}$$

and the corresponding optimal probability is equivalent to Eq. (A11).

Case 2.2.3 $p_1^+\leq 0$ or $p_1^-\geq 1$.

If $p_1^+\leq 0$, which is equivalent to

$$\alpha_{22}<0, x^2+y^2<x_2^2+y_2^2, \tag{A19}$$

the optimal distance

$$D^{\rm opt}(\rho,\chi)=\sqrt{x_2^2+y_2^2}-\sqrt{x^2+y^2}, \tag{A20}$$

and the corresponding optimal probability

$$p_1^{\rm opt}=0,\ \ p_2^{\rm opt}=1, \tag{A21}$$

which is located at the boundary of the constraint conditions.

If $p_1^-\geq 1$, which is equivalent to

$$\alpha_{11}<0,\ \ x^2+y^2<x_1^2+y_1^2, \tag{A22}$$

the optimal distance

$$D^{\rm opt}(\rho,\chi)=\sqrt{x_1^2+y_1^2}-\sqrt{x^2+y^2}, \tag{A23}$$

and the corresponding optimal probability

$$p_1^{\rm opt}=1,\ \ p_2^{\rm opt}=0, \tag{A24}$$

which is located at the boundary of the constraint conditions.

To sum up, we have shown that in every case, the optimal value is just given by Eqs. (6)–(22), which completes the proof.

Appendix B: The given quantum state parameter range of Theorem 2

Consider the number $N=3$ of quantum states in the given set $\{S\}$. We can specify the following regions:

$$\begin{aligned}&①:\alpha_{11}+\alpha_{33}\neq 0,\ \beta_{22}+\beta_{33}\neq 0,\ c_{12}\neq 0,\ \tau\neq 0,\\&②:\frac{-\alpha_{13}}{\tau}-\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)}}{|\tau|}\leq p_2\\&\qquad\leq\frac{-\alpha_{13}}{\tau}+\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)}}{|\tau|},\\&③:x_{123}+\alpha_{33}=0,\ \ ④:x_{123}+\alpha_{33}\neq 0,\\&⑤:\alpha_{33}\geq 0,\end{aligned} \tag{B1}$$

$$
\begin{aligned}
&⑥: \alpha_{33}<0,\ x^2+y^2 \geq \frac{\alpha_{33}^2}{\alpha_{11}+\alpha_{33}},\\
&\quad \frac{-\alpha_{13}}{\tau}-\Delta_{33} \leq p_2 \leq \frac{-\alpha_{13}}{\tau}+\Delta_{33}.\\
&⑦: \alpha_{11}\geq 0,\ x^2+y^2 \leq \frac{\alpha_{11}^2}{\alpha_{11}+\alpha_{33}},\\
&⑧: \alpha_{11}\geq 0,\ \ x^2+y^2 \geq \frac{\alpha_{11}^2}{\alpha_{11}+\alpha_{33}},\\
&\quad p_2 \leq \frac{-\alpha_{13}}{\tau}-\Delta_{11} \cup p_2 \geq \frac{-\alpha_{13}}{\tau}+\Delta_{11}, \qquad \text{(B2)}\\
&⑨: \alpha_{11}\geq 0,\\
&⑩: \alpha_{11}<0,\ x^2+y^2 \geq \frac{\alpha_{11}^2}{\alpha_{11}+\alpha_{33}},\\
&\quad \frac{-\alpha_{13}}{\tau}-\Delta_{11} \leq p_2 \leq \frac{-\alpha_{13}}{\tau}+\Delta_{11},\\
&⑪: \alpha_{33}\geq 0,\ x^2+y^2 \leq \frac{\alpha_{33}^2}{\alpha_{11}+\alpha_{33}},\\
&⑫: \alpha_{33}\geq 0,\ \ x^2+y^2 > \frac{\alpha_{33}^2}{\alpha_{11}+\alpha_{33}},\\
&\quad p_2 \leq \frac{-\alpha_{13}}{\tau}-\Delta_{33} \cup p_2 \geq \frac{-\alpha_{13}}{\tau}+\Delta_{33}, \qquad \text{(B3)}\\
&⑬: x_{123}+\alpha_{33}>0,\ \alpha_{33}\geq 0,\ p_2 \leq \frac{\alpha_{33}}{x_{123}+\alpha_{33}},\\
&⑭: x_{123}+\alpha_{33}<0,\ x_{123}\leq 0,\ p_2 \geq \frac{\alpha_{33}}{x_{123}+\alpha_{33}},\\
&⑮: x_{123}+\alpha_{33}>0,\ x_{123}>0,\ p_2 > \frac{\alpha_{33}}{x_{123}+\alpha_{33}},\\
&⑯: x_{123}+\alpha_{33}<0,\ \alpha_{33}<0,\ p_2 < \frac{\alpha_{33}}{x_{123}+\alpha_{33}},\\
&⑰: x^2+y^2 \geq \frac{\beta_{23}^2}{\beta_{22}+\beta_{33}},\\
&\quad \frac{\beta_{33}}{\beta_{22}+\beta_{33}}-\Delta_{23} \leq p_2 \leq \frac{\beta_{33}}{\beta_{22}+\beta_{33}}+\Delta_{23}, \qquad \text{(B4)}\\
&⑱: x_{123}+\alpha_{33}>0,\ \ x_{123}+\alpha_{11}+\alpha_{33}\geq 0,\\
&\quad p_2 \geq \frac{-\alpha_{11}}{x_{123}+\alpha_{33}},\\
&⑲: x_{123}+\alpha_{33}<0,\ \alpha_{11}>0,\ p_2 < \frac{-\alpha_{11}}{x_{123}+\alpha_{33}}.\\
&⑳: x^2+y^2 \leq \frac{(\beta_{23}-\tau)^2}{\beta_{22}+\beta_{33}},\\
&㉑: x^2+y^2 > \frac{(\beta_{23}-\tau)^2}{\beta_{22}+\beta_{33}},\\
&\quad p_2 \leq \frac{-y_{123}}{\beta_{22}+\beta_{33}}-\Delta_{23\tau} \cup p_2 \geq \frac{-y_{123}}{\beta_{22}+\beta_{33}}+\Delta_{23\tau},\\
&㉒: x^2+y^2 \leq \frac{\beta_{23}^2}{\beta_{22}+\beta_{33}},\\
&㉓: x^2+y^2 > \frac{\beta_{23}^2}{\beta_{22}+\beta_{33}},\\
&\quad p_2 \leq \frac{\beta_{33}}{\beta_{22}+\beta_{33}}-\Delta_{23} \cup p_2 \geq \frac{\beta_{33}}{\beta_{22}+\beta_{33}}+\Delta_{23}, \qquad \text{(B5)}\\
&㉔: x_{123}+\alpha_{33}>0,\ \ x_{123}+\alpha_{11}+\alpha_{33}\geq 0,\\
&\quad p_2 \geq \frac{-\alpha_{11}}{x_{123}+\alpha_{33}},\\
&㉕: x_{123}+\alpha_{33}<0,\ \ \alpha_{11}\geq 0,\ \ p_2 \leq \frac{-\alpha_{11}}{x_{123}+\alpha_{33}},\\
&㉖: x_{123}+\alpha_{33}>0,\ \ \alpha_{11}<0,\ \ p_2 < \frac{-\alpha_{11}}{x_{123}+\alpha_{33}},\\
&㉗: x_{123}+\alpha_{33}<0,\ \ x_{123}+\alpha_{11}+\alpha_{33}<0,\\
&\quad p_2 > \frac{-\alpha_{11}}{x_{123}+\alpha_{33}},\\
&㉘: x^2+y^2 \geq \frac{(\beta_{23}-\tau)^2}{\beta_{22}+\beta_{33}},\\
&\quad \frac{-y_{123}}{\beta_{22}+\beta_{33}}-\Delta_{23\tau} \leq p_2 \leq \frac{-y_{123}}{\beta_{22}+\beta_{33}}+\Delta_{23\tau} \qquad \text{(B6)}
\end{aligned}
$$

with

$$
\begin{aligned}
&\tau = x_1(y_2-y_3)+x_2(y_3-y_1)+x_3(y_1-y_2),\\
&\alpha_{13} = x_1y_3-x_3y_1,\\
&\alpha_{11} = x_1(x_1-x_3)+y_1(y_1-y_3),\\
&\alpha_{33} = x_3(x_3-x_1)+y_3(y_3-y_1),\\
&x_{123} = x_2(x_1-x_3)+y_2(y_1-y_3), \qquad \text{(B7)}\\
&\beta_{23} = x_2y_3-x_3y_2,\\
&\beta_{22} = x_2(x_2-x_3)+y_2(y_2-y_3),\\
&\beta_{33} = x_3(x_3-x_2)+y_3(y_3-y_2),\\
&y_{123} = x_1(x_2-x_3)+y_1(y_2-y_3),\\
&c_{12} = (x_1-x_2)^2+(y_1-y_2)^2, \qquad \text{(B8)}\\
&\Delta_{11} = \frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{11}^2}}{|\tau|},\\
&\Delta_{33} = \frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{33}^2}}{|\tau|},\\
&\Delta_{23} = \frac{\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-\beta_{23}^2}}{\beta_{22}+\beta_{33}},\\
&\Delta_{23\tau} = \frac{\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-(\beta_{23}-\tau)^2}}{\beta_{22}+\beta_{33}}. \qquad \text{(B9)}
\end{aligned}
$$

Appendix C: Proof of Theorem 2

Consider the number $N=3$ of quantum states in the given set $\{S\}$. For $N=3$, equation (4) can be specifically rewritten as

$$D^{\text{opt}}(\rho,\chi) = \min_{\{p_1,p_2,p_3\}} \left|\sqrt{x^2+y^2}-\sqrt{Q(p_1,p_2,p_3)}\right|. \qquad \text{(C1)}$$

with $Q(p_1,p_2,p_3) = (p_1x_1+p_2x_2+p_3x_3)^2+(p_1y_1+p_2y_2+p_3y_3)^2$. For convenience, we set

$$\tau = x_1(y_2-y_3)+x_2(y_3-y_1)+x_3(y_1-y_2),$$

$$
\begin{aligned}
&\alpha_{13} = x_1y_3 - x_3y_1,\\
&\alpha_{11} = x_1(x_1-x_3)+y_1(y_1-y_3),\\
&\alpha_{33} = x_3(x_3-x_1)+y_3(y_3-y_1),\\
&x_{123} = x_2(x_1-x_3)+y_2(y_1-y_3),
\end{aligned}
\tag{C2}
$$

$$
\begin{aligned}
&\beta_{23} = x_2y_3 - x_3y_2,\\
&\beta_{22} = x_2(x_2-x_3)+y_2(y_2-y_3),\\
&\beta_{33} = x_3(x_3-x_2)+y_3(y_3-y_2),\\
&y_{123} = x_1(x_2-x_3)+y_1(y_2-y_3),\\
&c_{12} = (x_1-x_2)^2+(y_1-y_2)^2.
\end{aligned}
\tag{C3}
$$

Case 1 $\alpha_{11}+\alpha_{33}=0$ or $\beta_{22}+\beta_{33}=0$ or $c_{12}=0$.

In this case, we have $x_1=x_2$, $y_1=y_2$ or $x_2=x_3$, $y_2=y_3$ or $x_1=x_2$, $y_1=y_2$. Since the x and y Bloch directions of two quantum states are the same, the effects of these two quantum states in the optimal coherence approximation are completely identical. That is to say, the optimal coherence approximation of three quantum states is equivalent to the optimal coherence approximation of two quantum states with different x or y Bloch directions, and its analytical solution lies at the boundary of the constraint conditions

$$
D^{\mathrm{opt}}(\rho,\chi) = \min\{D(p_1=0), D(p_2=0), D(p_3=0)\}, \tag{C4}
$$

which can be solved using Theorem 1.

Case 2 $\alpha_{11}+\alpha_{33}\neq 0$ and $\beta_{22}+\beta_{33}\neq 0$ and $c_{12}\neq 0$.

Case 2.1 $\tau=0$.

The condition $\tau=0$ implies that the three points $(x_1,y_1),(x_2,y_2),(x_3,y_3)$ in Euclidean space are collinear. Or, assuming that (x_2,y_2) is located between the other two points, then there exists a real number $\lambda\in[0,1]$ such that $(x_2,y_2)=\lambda(x_1,y_1)+(1-\lambda)(x_3,y_3)$. If $\boldsymbol{p}^{\mathrm{opt}}=\left(p_1^{\mathrm{opt}},p_2^{\mathrm{opt}},p_3^{\mathrm{opt}}\right)^{\mathrm{T}}$ is the optimal probability vector we need, then $\boldsymbol{p}^{\mathrm{opt}}=\left(p_1^{\mathrm{opt}}+\lambda p_2^{\mathrm{opt}},0,p_3^{\mathrm{opt}}+(1-\lambda)p_2^{\mathrm{opt}}\right)^{\mathrm{T}}$ is also the optimal probability vector, and the quantum states corresponding to the two have the same l_1-norm of coherence. Therefore, the optimal coherence approximation of the three quantum states in this case can also be equivalent to the optimal coherence approximation of two of the quantum states, which can be specifically expressed as Eq. (C4).

Case 2.2 $\tau\neq 0$.

Considering that the function $Q(p_1,p_2,p_3)=(p_1x_1+p_2x_2+p_3x_3)^2+(p_1y_1+p_2y_2+p_3y_3)^2$ is a convex function, its minimum value without the constraint that $p_n\in[0,1]$ is located at

$$
p_1=\frac{\beta_{23}}{\tau},\quad p_2=\frac{-\alpha_{13}}{\tau},\quad p_3=\frac{x_1y_2-x_2y_1}{\tau}, \tag{C5}
$$

$$
Q_{\min}(p_1,p_2,p_3)=0. \tag{C6}
$$

This means that the function $Q_1=x^2+y^2$ and the function Q always have intersection points, even when we do not consider the constraint conditions $p_n\in[0,1]$. Next, we will start to solve the analytical solutions of the intersection points. In other words, we consider the situation where the optimal distance is zero, that is to say,

$$
\begin{aligned}
&F(p_1,p_2,p_3)\\
&= Q(p_1,p_2,p_3)-(x^2+y^2)\\
&= p_1^2[(x_1-x_3)^2+(y_1-y_3)^2]+[p_2(x_2-x_3)+x_3]^2\\
&\quad +[p_2(y_2-y_3)+y_3]^2-(x^2+y^2)\\
&\quad +2p_1[p_2(x_1-x_3)(x_2-x_3)+p_2(y_1-y_3)(y_2-y_3)\\
&\quad +x_3(x_1-x_3)+y_3(y_1-y_3)]=0.
\end{aligned}
\tag{C7}
$$

The solution to the above equation is

$$
p_1^{\pm}=\frac{-p_2(x_{123}+\alpha_{33})+\alpha_{33}\pm\sqrt{\Delta}}{\alpha_{11}+\alpha_{33}} \tag{C8}
$$

with $\Delta=(\alpha_{11}+\alpha_{33})(x^2+y^2)-(p_2\tau+\alpha_{13})^2$. Our focus of calculation has now shifted the selection of an appropriate parameter $p_2\in[0,1]$ so that p_1 falls within the constraint range of zero to one, thereby obtaining a result with an optimal distance of zero.

A necessary condition for $p_1^{\pm}\in[0,1]$ in Eq. (C8) is $\Delta\geq 0$, which can be rewritten as

$$
(p_2\tau+\alpha_{13})^2\leq(\alpha_{11}+\alpha_{33})(x^2+y^2) \tag{C9}
$$

and further written as

$$
p_2\geq\frac{-\alpha_{13}}{\tau}-\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)}}{|\tau|}, \tag{C10}
$$

$$
p_2\leq\frac{-\alpha_{13}}{\tau}+\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)}}{|\tau|}. \tag{C11}
$$

The premise under which Eq. (C10) is meaningful is that

$$
\frac{-\alpha_{13}}{\tau}-\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)}}{|\tau|}\leq 1, \tag{C12}
$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$
\tau(\tau+\alpha_{13})\geq 0, \tag{C13}
$$

or

$$
\tau(\tau+\alpha_{13})<0,\ \ x^2+y^2\geq\frac{(\tau+\alpha_{13})^2}{\alpha_{11}+\alpha_{33}}. \tag{C14}
$$

Similarly, the premise under which Eq. (C11) is meaningful is that

$$
\frac{-\alpha_{13}}{\tau}+\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)}}{|\tau|}\geq 0, \tag{C15}
$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$
\tau\alpha_{13}\leq 0, \tag{C16}
$$

or

$$\tau\alpha_{13} > 0,\ \ x^2+y^2 \geq \frac{\alpha_{13}^2}{\alpha_{11}+\alpha_{33}}. \tag{C17}$$

To sum up, Eqs. (C10)–(C17) are the prerequisite conditions for the function $\Delta \geq 0$. All the situations we discuss next are based on this.

Case 2.2.1 $\Delta \geq 0,\ x_{123}+\alpha_{33}=0$.

In this case, equation (C8) can be rewritten as

$$p_1^{\pm} = \frac{\alpha_{33} \pm \sqrt{\Delta}}{\alpha_{11}+\alpha_{33}}. \tag{C18}$$

Case 2.2.1.1 $0 \leq p_1^+ \leq 1$.

The equivalent condition for $p_1^+ \geq 0$ is

$$\alpha_{33} \geq 0, \tag{C19}$$

or

$$\alpha_{33} < 0,\ (p_2\tau+\alpha_{13})^2 \leq (\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{33}^2. \tag{C20}$$

The above Eq. (C20) can be further calculated using

$$x^2+y^2 \geq \frac{\alpha_{33}^2}{\alpha_{11}+\alpha_{33}}, \tag{C21}$$

$$p_2 \geq \frac{-\alpha_{13}}{\tau} - \frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{33}^2}}{|\tau|}, \tag{C22}$$

$$p_2 \leq \frac{-\alpha_{13}}{\tau} + \frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{33}^2}}{|\tau|}. \tag{C23}$$

The premise under which Eq. (C22) is meaningful is that

$$\frac{-\alpha_{13}}{\tau} - \frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{33}^2}}{|\tau|} \leq 1, \tag{C24}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$\tau(\tau+\alpha_{13}) \geq 0, \tag{C25}$$

or

$$\tau(\tau+\alpha_{13}) < 0,\ \ x^2+y^2 \geq \frac{(\tau+\alpha_{13})^2+\alpha_{33}^2}{\alpha_{11}+\alpha_{33}}. \tag{C26}$$

Similarly, the premise under which Eq. (C23) is meaningful is that

$$\frac{-\alpha_{13}}{\tau} + \frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{33}^2}}{|\tau|} \geq 0, \tag{C27}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$\tau\alpha_{13} \leq 0, \tag{C28}$$

or

$$\tau\alpha_{13} > 0,\ \ x^2+y^2 \geq x_3^2+y_3^2. \tag{C29}$$

The equivalent condition for $p_1^+ \leq 1$ is

$$\alpha_{11} \geq 0,\ \ (p_2\tau+\alpha_{13})^2 \geq (\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{11}^2. \tag{C30}$$

The solutions of the above Eq. (C30) are distributed over two regions. The first region is

$$x^2+y^2 \leq \frac{\alpha_{11}^2}{\alpha_{11}+\alpha_{33}}, \tag{C31}$$

and the second region is

$$x^2+y^2 > \frac{\alpha_{11}^2}{\alpha_{11}+\alpha_{33}}, \tag{C32}$$

$$p_2 \geq \frac{-\alpha_{13}}{\tau} + \frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{11}^2}}{|\tau|}, \tag{C33}$$

$$p_2 \leq \frac{-\alpha_{13}}{\tau} - \frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{11}^2}}{|\tau|}. \tag{C34}$$

The premise under which Eq. (C33) is meaningful is that

$$\frac{-\alpha_{13}}{\tau} + \frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{11}^2}}{|\tau|} \leq 1, \tag{C35}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$\tau(\tau+\alpha_{13}) \geq 0,\ \ x^2+y^2 \leq \frac{(\tau+\alpha_{13})^2+\alpha_{11}^2}{\alpha_{11}+\alpha_{33}}. \tag{C36}$$

Similarly, the premise under which Eq. (C34) is meaningful is that

$$\frac{-\alpha_{13}}{\tau} - \frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{11}^2}}{|\tau|} \geq 0, \tag{C37}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is or

$$\tau\alpha_{13} \leq 0,\ \ x^2+y^2 \leq x_1^2+y_1^2. \tag{C38}$$

To sum up, the necessary condition for $p_1^+ \geq 0$ in Case 2.2.1 is the Eqs. {(C19)}∪{(C20)∩(C21)∩[(C25)∪(C26)]∩[(C28)∪(C29)]}, the necessary condition for $p_1^+ \leq 1$ in Case 2.2.1 is the Eqs. {(C30)}∩{(C31)∪[(C32)∩(C36)∩(C38)]}, and the necessary condition for achieving an optimal distance of zero is that both conditions are met, that is $0 \leq p_1^+ \leq 1$.

Case 2.2.1.2 $0 \leq p_1^- \leq 1$.

The equivalent condition for $p_1^- \geq 0$ is

$$\alpha_{33} \geq 0,\ (p_2\tau+\alpha_{13})^2 \geq (\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{33}^2. \tag{C39}$$

The solutions of the above Equation (C39) are distributed over two regions. The first region is

$$x^2+y^2 \leq \frac{\alpha_{33}^2}{\alpha_{11}+\alpha_{33}}, \tag{C40}$$

and the second region is

$$x^2+y^2>\frac{\alpha_{33}^2}{\alpha_{11}+\alpha_{33}}, \tag{C41}$$

$$p_2\geq\frac{-\alpha_{13}}{\tau}+\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{33}^2}}{|\tau|}, \tag{C42}$$

$$p_2\leq\frac{-\alpha_{13}}{\tau}-\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{33}^2}}{|\tau|}. \tag{C43}$$

The premise under which Eq. (C42) is meaningful is that

$$\frac{-\alpha_{13}}{\tau}+\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{33}^2}}{|\tau|}\leq 1, \tag{C44}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$\tau(\tau+\alpha_{13})\geq 0,\ \ x^2+y^2\leq\frac{(\tau+\alpha_{13})^2+\alpha_{33}^2}{\alpha_{11}+\alpha_{33}}. \tag{C45}$$

Similarly, the premise under which Eq. (C43) is meaningful is that

$$\frac{-\alpha_{13}}{\tau}-\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{33}^2}}{|\tau|}\geq 0, \tag{C46}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$\tau\alpha_{13}\leq 0,\ \ x^2+y^2\leq x_3^2+y_3^2. \tag{C47}$$

The equivalent condition for $p_1^-\leq 1$ is

$$\alpha_{11}\geq 0, \tag{C48}$$

or

$$\alpha_{11}<0,\ (p_2\tau+\alpha_{13})^2\leq(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{11}^2. \tag{C49}$$

The above Eq. (C49) can be further calculated using

$$x^2+y^2\geq\frac{\alpha_{11}^2}{\alpha_{11}+\alpha_{33}}, \tag{C50}$$

$$p_2\geq\frac{-\alpha_{13}}{\tau}-\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{11}^2}}{|\tau|}, \tag{C51}$$

$$p_2\leq\frac{-\alpha_{13}}{\tau}+\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{11}^2}}{|\tau|}. \tag{C52}$$

The premise under which Eq. (C51) is meaningful is that

$$\frac{-\alpha_{13}}{\tau}-\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{11}^2}}{|\tau|}\leq 1, \tag{C53}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$\tau(\tau+\alpha_{13})\geq 0, \tag{C54}$$

or

$$\tau(\tau+\alpha_{13})<0,\ \ x^2+y^2\geq\frac{(\tau+\alpha_{13})^2+\alpha_{11}^2}{\alpha_{11}+\alpha_{33}}. \tag{C55}$$

Similarly, the premise under which Eq. (C52) is meaningful is that

$$\frac{-\alpha_{13}}{\tau}+\frac{\sqrt{(\alpha_{11}+\alpha_{33})(x^2+y^2)-\alpha_{11}^2}}{|\tau|}\geq 0, \tag{C56}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$\tau\alpha_{13}\leq 0, \tag{C57}$$

or

$$\tau\alpha_{13}>0,\ \ x^2+y^2\geq x_1^2+y_1^2. \tag{C58}$$

To sum up, the necessary condition for $p_1^-\geq 0$ in Case 2.2.1 is Eqs. $\{(C39)\}\cap\{(C40)\cup[(C41)\cap(C45)\cap(C47)]\}$, the necessary condition for $p_1^-\leq 1$ in Case 2.2.1 is Eqs. $\{(C48)\}\cup\{(C49)\cap(C50)\cap[(C54)\cup(C55)]\cap[(C57)\cup(C58)]\}$, and the necessary condition for achieving an optimal distance of zero is that both conditions are met, that is $0\leq p_1^-\leq 1$.

Case 2.2.2 $\Delta\geq 0, x_{123}+\alpha_{33}\neq 0$.

Similarly, we calculate the ranges of the Bloch vectors of the given quantum state when $p_1^{\pm}$ in Eq. (C8) are within the constraint conditions.

Case 2.2.2.1 $0\leq p_1^+\leq 1$.

The equivalent condition for $p_1^+\geq 0$ is

$$p_2(x_{123}+\alpha_{33})-\alpha_{33}\leq\sqrt{\Delta}, \tag{C59}$$

and its solutions are distributed over the following two regions. The first region is

$$p_2(x_{123}+\alpha_{33})-\alpha_{33}\leq 0, \tag{C60}$$

which can be further written as

$$x_{123}+\alpha_{33}>0,\ \ \alpha_{33}\geq 0, \tag{C61}$$

$$p_2\leq\frac{\alpha_{33}}{x_{123}+\alpha_{33}}, \tag{C62}$$

or

$$x_{123}+\alpha_{33}<0,\ \ x_{123}\leq 0, \tag{C63}$$

$$p_2\geq\frac{\alpha_{33}}{x_{123}+\alpha_{33}}. \tag{C64}$$

The second region is

$$p_2(x_{123}+\alpha_{33})-\alpha_{33}>0. \tag{C65}$$

which can be further written as

$$x_{123}+\alpha_{33}>0,\ \ x_{123}>0, \tag{C66}$$

$$p_2 > \frac{\alpha_{33}}{x_{123}+\alpha_{33}}, \tag{C67}$$

or

$$x_{123}+\alpha_{33} < 0, \ \ \alpha_{33} < 0, \tag{C68}$$

$$p_2 < \frac{\alpha_{33}}{x_{123}+\alpha_{33}}. \tag{C69}$$

In this region, equation (C59) implies that

$$\begin{aligned} Q_2(p_2) \ = \ & p_2^2(\beta_{22}+\beta_{33}) - 2p_2\beta_{33} \\ & +x_3^2+y_3^2-x^2-y^2 \le 0, \end{aligned} \tag{C70}$$

which can be further written as

$$x^2+y^2 \ge \frac{\beta_{23}^2}{\beta_{22}+\beta_{33}}, \tag{C71}$$

$$p_2 \ge \frac{\beta_{33}-\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-\beta_{23}^2}}{\beta_{22}+\beta_{33}}, \tag{C72}$$

$$p_2 \le \frac{\beta_{33}+\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-\beta_{23}^2}}{\beta_{22}+\beta_{33}}. \tag{C73}$$

The premise under which Eq. (C72) is meaningful is that

$$\frac{\beta_{33}-\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-\beta_{23}^2}}{\beta_{22}+\beta_{33}} \le 1, \tag{C74}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$\beta_{22} \ge 0, \tag{C75}$$

or

$$\beta_{22} < 0, \ \ x^2+y^2 \ge x_2^2+y_2^2. \tag{C76}$$

Similarly, the premise under which Eq. (C73) is meaningful is that

$$\frac{\beta_{33}+\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-\beta_{23}^2}}{\beta_{22}+\beta_{33}} \ge 0, \tag{C77}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$\beta_{33} \ge 0, \tag{C78}$$

or

$$\beta_{33} < 0, \ \ x^2+y^2 \ge x_3^2+y_3^2. \tag{C79}$$

The equivalent condition for $p_1^+ \le 1$ is

$$p_2(x_{123}+\alpha_{33})+\alpha_{11} \ge \sqrt{\Delta}, \tag{C80}$$

and its necessary condition is

$$p_2(x_{123}+\alpha_{33})+\alpha_{11} \ge 0, \tag{C81}$$

which can be further written as

$$x_{123}+\alpha_{33} > 0, \ \ x_{123}+\alpha_{11}+\alpha_{33} \ge 0, \tag{C82}$$

$$p_2 \ge \frac{-\alpha_{11}}{x_{123}+\alpha_{33}}, \tag{C83}$$

or

$$x_{123}+\alpha_{33} < 0, \ \ \alpha_{11} > 0, \tag{C84}$$

$$p_2 < \frac{-\alpha_{11}}{x_{123}+\alpha_{33}}. \tag{C85}$$

In this case, equation (C80) implies that

$$\begin{aligned} Q_3(p_2) \ = \ & p_2^2(\beta_{22}+\beta_{33}) + 2p_2y_{123} \\ & +x_1^2+y_1^2-x^2-y^2 \ge 0, \end{aligned} \tag{C86}$$

and its solutions are distributed over the following two regions. The first region is

$$x^2+y^2 \le \frac{(\beta_{23}-\tau)^2}{\beta_{22}+\beta_{33}}, \tag{C87}$$

which implies that the minimum value of the function Q_3 is zero. The second region is

$$x^2+y^2 > \frac{(\beta_{23}-\tau)^2}{\beta_{22}+\beta_{33}}, \tag{C88}$$

$$p_2 \ge \frac{-y_{123}+\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-(\beta_{23}-\tau)^2}}{\beta_{22}+\beta_{33}}, \tag{C89}$$

$$p_2 \le \frac{-y_{123}-\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-(\beta_{23}-\tau)^2}}{\beta_{22}+\beta_{33}}. \tag{C90}$$

The premise under which equation (C89) is meaningful is that

$$\frac{-y_{123}+\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-(\beta_{23}-\tau)^2}}{\beta_{22}+\beta_{33}} \le 1, \tag{C91}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$\begin{aligned} & \beta_{22}+\beta_{33}+y_{123} \ge 0, \\ & x^2+y^2 \le x_1^2+y_1^2+\beta_{22}+\beta_{33}+2y_{123}. \end{aligned} \tag{C92}$$

Similarly, the premise under which Eq. (C90) is meaningful is that

$$\frac{-y_{123}-\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-(\beta_{23}-\tau)^2}}{\beta_{22}+\beta_{33}} \ge 0, \tag{C93}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$y_{123} \le 0, \ \ x^2+y^2 \le x_1^2+y_1^2. \tag{C94}$$

To sum up, the necessary condition for $p_1^+ \ge 0$ in Case 2.2.2 is the Eqs. {(C61)∩(C64)}∪{[(C66)∪(C68)]∩(C71)∩[(C75)∪(C76)]∩[(C78)∪(C79)]}, the necessary condition for $p_1^+ \le 1$ in Case 2.2.2 is the Eqs. {(C82)∪(C84)}∩{(C87)∪[(C88)∩(C92)∩(C94)]}, and the necessary condition for achieving an

optimal distance of zero is that both conditions are met, that is $0 \leq p_1^+ \leq 1$.

Case 2.2.2.2 $0 \leq p_1^- \leq 1$.

The equivalent condition for $p_1^- \geq 0$ in Eq. (C8) is

$$p_2(x_{123}+\alpha_{33})-\alpha_{33} \leq -\sqrt{\Delta}, \tag{C95}$$

and its necessary condition is

$$p_2(x_{123}+\alpha_{33})-\alpha_{33} \leq 0, \tag{C96}$$

which can be further written as

$$x_{123}+\alpha_{33} > 0, \quad \alpha_{33} \geq 0, \tag{C97}$$

$$p_2 \leq \frac{\alpha_{33}}{x_{123}+\alpha_{33}}, \tag{C98}$$

or

$$x_{123}+\alpha_{33} < 0, \quad x_{123} \leq 0, \tag{C99}$$

$$p_2 \geq \frac{\alpha_{33}}{x_{123}+\alpha_{33}}. \tag{C100}$$

In this case, equation (C95) implies that

$$\begin{aligned} Q_4(p_2) \;=\; & p_2^2(\beta_{22}+\beta_{33})-2p_2\beta_{33} \\ & +x_3^2+y_3^2-x^2-y^2 \geq 0, \end{aligned} \tag{C101}$$

and its solutions are distributed over the following two regions. The first region is

$$x^2+y^2 \leq \frac{\beta_{23}^2}{\beta_{22}+\beta_{33}}, \tag{C102}$$

which implies that the minimum value of the function Q_4 is zero. The second region is

$$x^2+y^2 > \frac{\beta_{23}^2}{\beta_{22}+\beta_{33}}, \tag{C103}$$

$$p_2 \geq \frac{\beta_{33}+\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-\beta_{23}^2}}{\beta_{22}+\beta_{33}}, \tag{C104}$$

$$p_2 \leq \frac{\beta_{33}-\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-\beta_{23}^2}}{\beta_{22}+\beta_{33}}. \tag{C105}$$

The premise under which Eq. (C104) is meaningful is that

$$\frac{\beta_{33}+\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-\beta_{23}^2}}{\beta_{22}+\beta_{33}} \leq 1, \tag{C106}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$\beta_{22} \geq 0, \;\; x^2+y^2 \leq x_2^2+y_2^2. \tag{C107}$$

Similarly, the premise under which Eq. (C105) is meaningful is that

$$\frac{\beta_{33}-\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-\beta_{23}^2}}{\beta_{22}+\beta_{33}} \geq 0, \tag{C108}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$\beta_{33} \geq 0, \;\; x^2+y^2 \leq x_3^2+y_3^2. \tag{C109}$$

The equivalent condition for $p_1^- \leq 1$ is

$$p_2(x_{123}+\alpha_{33})+\alpha_{11} \geq -\sqrt{\Delta}, \tag{C110}$$

and its solutions are distributed over the following two regions. The first region is

$$p_2(x_{123}+\alpha_{33})+\alpha_{11} \geq 0, \tag{C111}$$

which can be further written as

$$x_{123}+\alpha_{33} > 0, \;\; x_{123}+\alpha_{11}+\alpha_{33} \geq 0, \tag{C112}$$

$$p_2 \geq \frac{-\alpha_{11}}{x_{123}+\alpha_{33}}, \tag{C113}$$

or

$$x_{123}+\alpha_{33} < 0, \;\; \alpha_{11} \geq 0, \tag{C114}$$

$$p_2 \leq \frac{-\alpha_{11}}{x_{123}+\alpha_{33}}. \tag{C115}$$

The second region is

$$p_2(x_{123}+\alpha_{33})+\alpha_{11} < 0, \tag{C116}$$

which can be further written as

$$x_{123}+\alpha_{33} > 0, \;\; \alpha_{11} < 0, \tag{C117}$$

$$p_2 < \frac{-\alpha_{11}}{x_{123}+\alpha_{33}}, \tag{C118}$$

or

$$x_{123}+\alpha_{33} < 0, \;\; x_{123}+\alpha_{11}+\alpha_{33} < 0, \tag{C119}$$

$$p_2 > \frac{-\alpha_{11}}{x_{123}+\alpha_{33}}. \tag{C120}$$

In this region, equation (C110) implies that

$$\begin{aligned} Q_5(p_2) \;=\; & p_2^2(\beta_{22}+\beta_{33})+2p_2y_{123} \\ & +x_1^2+y_1^2-x^2-y^2 \leq 0, \end{aligned} \tag{C121}$$

which can be further written as

$$x^2+y^2 \geq \frac{(\beta_{23}-\tau)^2}{\beta_{22}+\beta_{33}}, \tag{C122}$$

$$p_2 \geq \frac{-y_{123}-\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-(\beta_{23}-\tau)^2}}{\beta_{22}+\beta_{33}}, \tag{C123}$$

$$p_2 \leq \frac{-y_{123}+\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-(\beta_{23}-\tau)^2}}{\beta_{22}+\beta_{33}}. \tag{C124}$$

The premise under which Eq. (C123) is meaningful is that

$$\frac{-y_{123}-\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-(\beta_{23}-\tau)^2}}{\beta_{22}+\beta_{33}}\leq 1, \quad \text{(C125)}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$y_{123}+\beta_{22}+\beta_{33}\geq 0, \quad \text{(C126)}$$

or

$$\begin{aligned} &y_{123}+\beta_{22}+\beta_{33}<0,\\ &x^2+y^2\geq x_1^2+y_1^2+2y_{123}+\beta_{22}+\beta_{33}. \end{aligned} \quad \text{(C127)}$$

Similarly, the premise under which Equation (C124) is meaningful is that

$$\frac{-y_{123}+\sqrt{(x^2+y^2)(\beta_{22}+\beta_{33})-(\beta_{23}-\tau)^2}}{\beta_{22}+\beta_{33}}\geq 0, \quad \text{(C128)}$$

which indicates that the parameter range of the Bloch vector of the given quantum state is

$$y_{123}\leq 0, \quad \text{(C129)}$$

or

$$y_{123}>0,\ \ x^2+y^2\geq x_1^2+y_1^2. \quad \text{(C130)}$$

To sum up, the necessary condition for $p_1^-\geq 0$ in Case 2.2.2 is the Eqs. {(C97)∪(C100)}∩{(C102)∪[(C103)∩(C107)∩(C109)]}, the necessary condition for $p_1^-\leq 1$ in Case 2.2.2 is the Eqs. {(C112)∩(C114)}∪{[(C117)∪(C119)]∩(C122)∩[(C126)∪(C127)]∩[(C129)∪(C130)]}, and the necessary condition for achieving an optimal distance of zero is that both conditions are met, that is $0\leq p_1^-\leq 1$.

It should be emphasized that the state parameters given here are just one of the necessary conditions for the optimal distance to be zero. To achieve an optimal distance of zero, the various value-taking conditions of p_2 also need to be satisfied simultaneously. For example, when the given state parameter conditions are the Eqs. {(C13)∩(C16)∩(C61)∩(C82)∩(C87)} and $\{\tau\neq 0,\alpha_{11}+\alpha_{33}\neq 0,\beta_{22}+\beta_{33}\neq 0,c_{12}\neq 0,x_{123}+\alpha_{33}\neq 0\}$, $p_2\in[0,1]$ needs to simultaneously satisfy the conditions of the Eqs. {(C10)∩(C11)∩(C62)∩(C83)}. When the given state parameter conditions are the Eqs. {(C14∩C16∩C68∩C71∩C75∩C78∩C84∩C88∩C92∩C94} and $\{\tau\neq 0,\alpha_{11}+\alpha_{33}\neq 0,\beta_{22}+\beta_{33}\neq 0,c_{12}\neq 0,x_{123}+\alpha_{33}\neq 0\}$, $p_2\in[0,1]$ needs to simultaneously satisfy the conditions of the Eqs. {(C10)∩(C11)∩(C69)∩(C72)∩(C73)∩(C85)∩[(C89)∪(C90)]}. If these conditions are compatible, then the optimal distance is zero. If these conditions are mutually contradictory, then p_2 cannot take values at this time, and the optimal distance can only be evaluated at the boundary conditions of the constraints (it may also be zero).

Case 2.2.3 $\Delta<0$.

In this case, the probability p_1 in Eqs. (C8) is a complex number that contradicts the true probability, so the optimal solution in this case is located at the boundary conditions, i.e., Eq. (C4).

We have previously discussed that selecting the appropriate parameter range of the Bloch vector of the quantum state can locate the intersection point of the functions $Q_1(x,y)$ and $Q(p_1,p_2,p_3)$ within the constraint condition $p_n\in[0,1]$. In this case, the optimal distance is zero, and the coherence of the target quantum state ρ can be fully prepared. For other parameter ranges of the Bloch vector, the intersection point of the functions $Q_1(x,y)$ and $Q(p_1,p_2,p_3)$ falls outside the constraint condition $p_n\in[0,1]$. In this case, we can determine the optimal value by selecting the boundary conditions of the constraint, which are given by Eq. (C4).

To sum up, we find that the optimal approximation situations for $N=3$ can mainly be divided into two categories. The first category is the parameter range $\alpha_{11}+\alpha_{33}\neq 0,\beta_{22}+\beta_{33}\neq 0,c_{12}\neq 0,\tau\neq 0,\Delta\geq 0$ and $\{p_1^{\pm},p_2,p_3\}\in[0,1]$ in Eq. (C8), and, in this case, the optimal distance can be taken to be zero under the optimal probability. The remaining parameter ranges belong to the second category. In this case, the optimal value is located at the boundary conditions, and the optimal distance is not necessarily zero. The proof is complete.

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