The optimal approximation of qubit states with limited quantum states

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Measuring the closest distance between two states is an alternative and significant approach in the resource quantification, which is the core task in the resource theory. Quite limited progress has been made for this approach even in simple systems due to the various potential complexities. Here we analytically solve the optimal scheme to find out the closest distance between the objective qubit state and all the possible states convexly mixed by some limited states, namely, to optimally construct the objective qubit state using the quantum states within any given state set. In particular, we find the least number of (not more than four) states within a given set to optimally construct the objective state and also find that any state can be optimally established by at most four quantum states of the set. The examples in various cases are presented to verify our analytic solutions further.

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Introduction.-Quantum mechanical intriguing features are the essential ingredients that distinguish the quantum and the classical worlds, and at the heart of the quantum information, because they can be exploited to achieve the quantum information processing tasks and hence serve as the unsubstitutable physical resources. The resource theory, which quantitatively characterizes the quantum features in a mathematically rigorous fashion, has been extensively developed in recent years [1–6]. There are two ingredients in a well-defined resource theory: the free states, which do not owe any quantum feature of interest, and the free operations, which cannot convert the free states to the resource states (opposite to the free states). Besides, a quantitative framework for any quantum feature also depends on how to discriminate the given state from the free states unambiguously [6–11].

The most remarkable example is the quantification of entanglement [12–17], which is essential to find the least distance between the given state and the separable-state set. Since the convex mixing of free states is still within the free-state set, the entanglement measure can also be regarded to find out the least distance between the given state and all potential convex mixings of separable states. Similarly, the quantum discord of a state can also be quantified by the distance from the closest convexed mixed local distinguishable states [5, 10–13, 18–25]. Besides, the widely studied coherence can be measured with the least distance from all the possible convex mixings of some given orthonormal basis [11–13, 27–34]. In this sense, the essential problem is to optimally approximate a given state by the convex mixing of the limited states.

The state approximation via the convex mixing of some limited states has its much more general significance. Suppose, in some particular experiment, one can only prepare the limited pure states whose set is denoted by \( \{ \psi_i \} \). But a general state \( \rho \) is required for some purpose. The question is, what is the best way to approximating the state \( \rho \) by the convex mixing of the states in set \( \{ \psi_i \} \) and how well the state \( \rho \) can be approximately replaced. Recently, the question has been addressed for some particular cases, such as approximating the given state by the eigenstates of several Pauli matrices based on various distance measures [35–37]. A related question was also considered for the optimal approximation of a desired and unavailable quantum channel \( \Phi \) by the convex mixing of a given set of other channels \( \{ \Phi_i \} \) [38–40].

In this paper, we analytically solve the optimal construction of a qubit state with the convex mixing of pure/mixed states subject to any given quantum state set [39–43]. We find the least number of states in a given set to optimally construct the objective state. In particular, we show that any qubit state can be optimally constructed by at most four states, no matter how many quantum states are given. Therefore, the optimal construction of a qubit state with more than four quantum states can be converted into the case with at most four quantum states, which is perfectly solved by the analytic and closed solution. In addition, we present some numerical and analytic examples to verify/demonstrate our analytic results.

The scheme.-Given a quantum state set \( S := \{ \rho_i, i = 1, 2, \ldots, N \} \) and an expected objective qubit state \( \rho \), the task is to prepare a state \( \sigma = \chi_{1, 2, \ldots, K} (\beta) = \sum_{i=1}^{K} p_i \rho_i \) by the convex mixing of \( K \leq N \) quantum states in the set \( S \) such that \( \sigma \) and \( \rho \) are as close as possible subject to the state distance

\[
D (\rho, \sigma) = \| \rho - \sigma \|_1 ,
\]

where \( \| X \|_1 \) is the trace norm with \( \| X \|_1 = \text{Tr} \sqrt{X^\dagger X} \). It is obvious that \( D (\rho, \sigma) \) is (joint) convex and contractive under trace-preserving quantum operation. \( D (\rho, \sigma) = 0 \) for \( \rho = \sigma \) and \( D (\rho, \sigma) = 2 \) for \( \rho \perp \sigma \). In addition, it is implied that only \( K \leq N \) states could achieve the optimal approximation of \( \rho \).
σ. For example, if the two eigenstates of ρ happened to be covered in the set $S$, ρ can be perfectly constructed by the two \((k = 2)\) states.

For a qubit state ρ, the trace norm between ρ and σ = χ₁₂,...,K (p̃) is given by

$$D(ρ, σ) = |λ₁| + |λ₂| = 2|λ₁|,$$

with λ₁ the eigenvalues of Hermitian matrix ρ − σ. In the Bloch representation, let $r_α$ denote the Bloch vector of ρ with its elements $r_{αα} = Tr(ρσ_α)$ and $r_k$ (rkα is its element) denote the Bloch vector of the kth state in $S$, where $σ_α$ are Pauli matrices with $α = x, y, z$. Then we get

$$D^2(ρ, σ) = \sum_{α,j} p_ip_j r_{αj} − 2p_i r_{αa} + r_{αa}^2.$$

Therefore, in the scheme, to construct the state σ close enough to the state ρ is equivalent to achieve $min_ρ D^2(ρ, χ₁₂,...,N (p̃))$.

It is obvious that the considered scheme is essentially an optimization problem. The Hessian matrix for this problem is defined by $H = \frac{∂^2 D^2}{∂ p^2}$, so one will immediately find that

$$H = \frac{∂ D^2}{∂ p^2} = 2R^T R,$$

with $R = (r₁, r₂, \ldots, r_N)$ being a \(3 \times N\) matrix. Then the optimized function $D^2(ρ, σ)$ is convex on p̃. It indicates that our considered scheme is a convex optimization problem \(\ref{1}\), which plays the dominant role in the optimal state construction. It allows us to find the optimal scheme on the boundaries of the constraints if the globally optimal points are beyond the constraints, which is the cornerstone of our whole letter.

The main results.-Now we can go forward to the optimal scheme by considering the different $N$, the number of the quantum states in the set $S$, in a rigorous way. Following these results below, one can directly find out the best way to approximately preparing a density matrix by any given quantum states, and the optimal distance between the prepared state and the objective state.

**Theorem 1.** Let the set $S$ contain two states \((N = 2)\). If $0 ≤ (r_o − r_2)^T (r_1 − r_2) ≤ ||r_1 − r_2||^2_2$, where $||r||^2_2 = √Tr^T r$, one can construct an optimal state $χ₁₂ (p̃)$ with the optimal distance given by

$$D^2(ρ, χ₁₂ (p̃)) = ||r_o − r_2||^2_2 − \frac{(r_o − r_2)^T (r_1 − r_2)^T}{||r_1 − r_2||^2_2}.$$

and the optimal weight p̃ given by

$$p_1 = \frac{(r_o − r_2)^T (r_1 − r_2)}{||r_1 − r_2||^2_2},
\quad p_2 = 1 − p_1.$$

If $(r_o − r_2)^T (r_1 − r_2) < 0$, the optimal distance is given by

$$D(ρ, χ₁₂ (p̃)) = D(ρ, χ₁₂ (p̃)) = ||r_o − r_2||_2.$$ \(\ref{7}\)

If $(r_o − r_2)^T (r_1 − r_2) > ||r_1 − r_2||^2_2$, the optimal distance is given by

$$D(ρ, χ₁₂ (p̃)) = D(ρ, χ₁₂ (p̃)) = ||r_o − r_1||_2.$$ \(\ref{8}\)

**Proof.** For $N = 2$, Eq. \(\ref{3}\) can be rewritten as

$$D^2(ρ, χ₁₂ (p̃)) = \sum_{ij} p_ip_j r_i^T r_j − 2p_i r_i^T r_o + r_o^T r_o.$$ \(\ref{9}\)

Consider the Lagrangian function

$$L(ρ, χ₁₂ (p̃)) = D^2(ρ, χ₁₂ (p̃)) − λ₁p_1 − λ₂p_2 + λ(p_1 + p_2 − 1),$$

where λ and λ₁ are the Lagrangian multipliers. The Karush-Kuhn-Tucker conditions \(\ref{10}\) are given by

$$\frac{∂L}{∂p_1} = 2p_1 r_1^T r_1 + 2p_2 r_i^T r_2 − 2r_o^T r_1 − λ₁ + λ = 0,$n$$

$$\frac{∂L}{∂p_2} = 2p_2 r_2^T r_2 + 2p_1 r_i^T r_2 − 2r_o^T r_2 − λ₂ + λ = 0,$n$$

$$λ_i p_i = 0, λ₁ ≥ 0, p_i ≥ 0, \sum p_i − 1 = 0.$$ \(\ref{11}\)

Solving above Eq. \(\ref{11}\) by $\frac{∂L}{∂p_1} − \frac{∂L}{∂p_2} = 0$, we have

$$2(p_1 r_1 + p_2 r_2)^T (r_1 − r_2) = 2r_o^T (r_1 − r_2) + λ₁ − λ₂,$n$$

$$p_1 + p_2 = 1.$$ \(\ref{12}\)

Then it will arrive at the valid $p_i$ as

$$p_1 = \frac{(r_o − r_2)^T (r_1 − r_2) + λ₁ − λ₂}{||r_1 − r_2||^2_2},$$

$$p_2 = 1 − p_1.$$ \(\ref{13}\)

If $0 ≤ (r_o − r_2)^T (r_1 − r_2) ≤ ||r_1 − r_2||^2_2$, we can get $λ₁ = λ₂ = 0$. Insert $p_i$ into $χ₁₂ (p̃)$, one will find

$$D^2(ρ, χ₁₂ (p̃)) = ||r_o − r_2||^2_2 − \frac{(r_o − r_2)^T (r_1 − r_2)^T}{||r_1 − r_2||^2_2}.$$ \(\ref{14}\)

If $(r_o − r_2)^T (r_1 − r_2) < 0$, we can get

$$λ₁ = \frac{−(r_o − r_2)^T (r_1 − r_2)}{||r_1 − r_2||^2_2},$$

$$p_2 = 1.$$ \(\ref{15}\)

The optimal distance is

$$D(ρ, χ₁₂ (p̃)) = ||r_o − r_2||_2.$$ \(\ref{16}\)
If \((r_o - r_2)^T (r_1 - r_2) > \|r_1 - r_2\|^2_2\), we can obtain
\[
p_1 = 1
\]
\[
\lambda_2 = \frac{(r_o - r_2)^T (r_1 - r_2)}{\|r_1 - r_2\|^2_2} - 1.
\] (17)

The optimal distance is
\[
D(\rho, \chi_{1,2} (\vec{p})) = \|r_o - r_1\|_2.
\] (18)

The proof is completed.

A special case of Theorem 1 is that the set \(S\) is made up of two orthonormal pure states \(|\varphi_1\rangle\) and \(|\varphi_2\rangle\). In this case, one can find that \(r_1^T r_2 = -1\) and \(2 r_o^T (r_1 - r_2) \leq 1 - r_1^T r_2\). Substituting these parameters into Theorem 1, one will directly obtain the optimal distance as
\[
D^2(\rho, \chi_{1,2} (\vec{p})) = r_o^T r_o - (r_1^T r_1)^2,
\] (19)
with \(i = 1, 2\) and the optimal weight as
\[
p_i = \frac{1}{2} (1 + r_o^T r_i).
\] (20)

In particular, \(r_o^T r_i = r_{oa}^2 r_{ia}\), if both \(|\varphi_1\rangle\) and \(|\varphi_2\rangle\) are the eigenstates of one Pauli matrix \(\sigma_{\alpha}\) with \(\alpha = x, y, z\), because the eigenstates of one Pauli matrix \(\sigma_{\alpha}\) lead to that \(\langle \varphi_i | \sigma_{\alpha} | \varphi_j \rangle = \pm 1\) and the vanishing average values on other Pauli matrices. Eq. (19) actually presents an alternative quantifier of coherence of the objective state \(\rho\) with respect to the basis defined by the two orthogonal pure states in \(S\), which coincides with the result in [44]. Besides, it is obvious that a quite neat result has been given for the case with only two states in \(S\). However, the cases for more than two states in the set \(S\) are much more complicated than that with \(N = 2\), which will be addressed in what follows.

**Theorem 2.** If there are three quantum states \((N = 3)\) in the set \(S\), one can construct a pseudo-state \(\chi_{1,2,3} (\vec{p})\) with the pseudo-probabilities as
\[
\tilde{p}_1 = \frac{1}{d} (-1)r_1^T (r_o - r_2)(r_2 - r_3)^T (r_o - r_2) - (r_2 - r_3)(r_o - r_2) (r_2 - r_3),
\] (21)
\[
\tilde{p}_2 = \frac{1}{d} (-1)r_1^T (r_o - r_3)(r_3 - r_1) (r_o - r_3) - (r_o - r_1)(r_o - r_3) (r_3 - r_1),
\] (22)
\[
\tilde{p}_3 = 1 - \tilde{p}_1 - \tilde{p}_2,
\] (23)
where
\[
d = \|r_1 - r_2\|^2_2 \|r_3 - r_2\|^2_2 - [(r_1 - r_2)^T (r_3 - r_2)]^2.
\] (24)

If \(\tilde{p}_i \geq 0\) holds for \(i = 1, 2, 3\), \(\chi_{1,2,3} (\vec{p})\) will be our expected optimal state with the optimal weights \(p_i = \tilde{p}_i\), and the optimal distance
\[
D^2(\rho, \chi_{1,2,3} (\vec{p})) = \sum_{i,j} p_i p_j r_i^T r_j - 2 p_i r_o^T r_i + r_o^T r_o.
\] (25)

Otherwise, the optimal state and the closest distance are given by
\[
D(\rho, \chi_{1,2,3} (\vec{p})) = \min_{i < j} D(\rho, \chi_{i,j} (\vec{p})), i, j = 1, 2, 3,
\] (26)
which as well as the corresponding weights can be solved by Theorem 1.

**Proof.** For \(N = 3\), one can substitute \(\chi_{1,2,3} (\vec{p})\) into \(D^2(\rho, \chi_{1,2,3} (\vec{p}))\) and establish the corresponding Lagrangian function as
\[
L(p_i, \lambda, \lambda_i) = \sum_{i,j} p_i p_j r_i^T r_j - 2 p_i r_o^T r_i + r_o^T r_o
\]
\[
- \sum_{i=1}^3 \lambda_i p_i + \lambda (\sum_{i=1}^3 p_i - 1),
\] (27)
where \(\lambda\) and \(\lambda_i\) are the Lagrangian multipliers. The Karush-Kuhn-Tucker conditions are given by
\[
\frac{\partial L}{\partial p_i} = 2 \sum_{j=1}^3 p_j r_i^T r_j - 2 r_o^T r_i + \lambda - \lambda_i = 0,
\] (28)
\[
\lambda_i \geq 0, p_i \geq 0, \lambda, \lambda_i = 0, i = 1, 2, 3.
\]
Solving Eq. (28) by \(\frac{\partial L}{\partial p_i} - \frac{\partial L}{\partial \lambda} = 0\) and \(\frac{\partial L}{\partial p_i} - \frac{\partial L}{\partial \lambda_i} = 0\), we have
\[
2 (p_1 r_1 + p_2 r_2 + p_3 r_3 - r_o)^T (r_1 - r_3) = \lambda_1 - \lambda_3,
\]
\[
2 (p_1 r_1 + p_2 r_2 + p_3 r_3 - r_o)^T (r_2 - r_3) = \lambda_2 - \lambda_3,
\]
\[
p_1 + p_2 + p_3 = 1.
\] (29)

We rewrite Eq. (26) in matrix form \(AP = B\) with
\[
A = \begin{pmatrix}
  r_1^T (r_1 - r_3) & r_2^T (r_1 - r_3) & r_3^T (r_1 - r_3) \\
  r_1^T (r_2 - r_3) & r_2^T (r_2 - r_3) & r_3^T (r_2 - r_3) \\
  1 & 1 & 1
\end{pmatrix},
\] (30)
\[
P = \begin{pmatrix}
  \tilde{p}_1 & \tilde{p}_2 & \tilde{p}_3
\end{pmatrix}^T,
\]
\[
B = \begin{pmatrix}
  r_o^T (r_1 - r_3) + \frac{1}{2} (\lambda_1 - \lambda_3) \\
  r_o^T (r_2 - r_3) + \frac{1}{2} (\lambda_2 - \lambda_3) \\
  1
\end{pmatrix}.
\] (31)

The determinant of matrix \(A\) is
\[
d = \|r_1 - r_2\|_2^2 \|r_3 - r_2\|_2^2 - [(r_1 - r_2)^T (r_3 - r_2)]^2.
\] (32)

**Case 1:** \(d = 0\). The determinant \(d = 0\) is equivalent to
\[
r_1 - r_2 = \Delta (r_3 - r_2)
\] (33)
where \(\Delta\) is an arbitrary constant. Thus only two independent equations in Eq. (29) are left. We can always let some \(p_i = 0\) in \(P\). So the left two nonvanishing \(p_i\) just correspond to the case of Theorem 1, and then we can choose the smallest one as
\[
\min_{i < j} D(\rho, \chi_{i,j} (\vec{p})), i, j = 1, 2, 3.
\] (34)
which can be exactly solved by Theorem 1.

**Case 2:** $d \neq 0$. By calculating $P = A^{-1}B$, we can get

$$p_1 = \tilde{p}_1 + \frac{b^T}{2d} [\lambda_1 b - \lambda_2 (a + b) + \lambda_3 a],$$
$$p_2 = \tilde{p}_2 + \frac{(a + b)^T}{2d} [-\lambda_1 b + \lambda_2 (a + b) - \lambda_3 a],$$
$$p_3 = \tilde{p}_3 + \frac{a^T}{2d} [\lambda_1 b - \lambda_2 (a + b) + \lambda_3 a].$$

(35)

with

$$\tilde{p}_1 = \frac{1}{d} [a^T (cb^T - bc^T)]b,$$
$$\tilde{p}_3 = \frac{1}{d} [a^T (ca^T - ac^T)]b,$$
$$\tilde{p}_2 = 1 - \tilde{p}_1 - \tilde{p}_3.$$  

(36)

and

$$a = r_1 - r_2, b = r_2 - r_3, c = r_o - r_2.$$  

(37)

If all $\tilde{p}_i \in [0, 1]$ for $i = 1, 2, 3$, then the optimal weights $p_i = \tilde{p}_i$. With the optimal weights $p_i$, one can calculate $\chi_{1,2,3}(\tilde{p}) = \sum_{i=1}^{3} p_i \rho_i$, and the optimal distance is hence given by $D(\rho, \chi_{1,2,3}(\tilde{p}))$. If not all $\tilde{p}_i \in [0, 1]$, the optimal weights should be on the boundaries which are described by (i) $p_1 = 0$, $\lambda_1 > 0$; (ii) $p_2 = 0$, $\lambda_2 > 0$; (iii) $p_3 = 0$, $\lambda_3 > 0$. In other words, there exists at least one $p_i = 0$ among the three. This corresponds to the case of Theorem 1 again. The final optimal distance is shown in Eq. (34). The proof is completed.

Theorem 2 shows some kind of degradation relation. That is, the validity of the pseudo-probabilities have to be evaluated first. Once the pseudo-probabilities are invalid, the problem with $N = 3$ will be reduced into the case with $N = 2$, which implies that one has to use theorem 2 three times to find the minimal value. Such a degradation relation ensures that Theorem 2 for $N = 2$ will be automatically reduced to Theorem 1. Next, we will focus on the case of $N = 4$. To do so, we will have to address the special case of full-rank $4 \times K$ matrix $A$, which is defined as $A_{i,j} = \text{Tr}(\sigma_i \rho_j)$ with $j = 1, 2, 3, \cdots, K$ and $i = 1, 2, 3, 4$ corresponding to $x, y, z,$ and $\sigma_4 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

**Theorem 3.** If there are four quantum states ($N = 4$) in the set $S$ with the rank-4 matrix $A$, one can obtain the exact objective state $\rho$ with the pseudo-probabilities

$$\tilde{p} = A^{-1} \tilde{r}.$$  

(38)

where $\tilde{r} = [r; 1]$ is a four-dimensional vector. If $\tilde{p}_j \in [0, 1]$ for all $j$, the objective state $\rho$ can be exactly written as the convex sum of the four quantum states with the optimal weights $p = \tilde{p}$. Otherwise, the optimal approximation can be solved based on Theorem 2 as

$$\min_{i \prec j \prec k} D(\rho, \chi_{i,j,k}(\tilde{p})),$$  

(39)

where $\tilde{p}$ is the convex mixing of the $R + 1$ columns of $A$, i.e., $\tilde{r}_o = \sum_{i=1}^{R+1} p_i A_i$ with $\sum_i p_i = 1$ and $\tilde{p}_i \geq 0$. Thus

**Proof.** The convex optimization guarantees an important property that if the optimal solutions of a problem with some constraints $S_1$ don’t satisfy the other constraints $S_2$, then the optimal solutions with the constraints $S_1 \cup S_2$ must be present on the boundaries of $S_2$. Now let’s suppose that the objective quantum state $\rho$ can be exactly expressed by the linear sum of the given four quantum states in $S$, then one will definitely find the pseudo-probabilities $\tilde{p}_i$ such that $\rho = \sum_{i=1}^{4} \tilde{p}_i \rho_i$ with $\sum \tilde{p}_i = 1$. Note that $\tilde{p}_i$ could be negative. Thus in the i-th Bloch representation, the above relation can be rewritten as

$$A \tilde{p} = \tilde{r}.$$  

(40)

with $\tilde{r} = [r; 1]$ and $\tilde{p} = (\tilde{p}_1, \tilde{p}_2, \tilde{p}_3, \tilde{p}_4)^T$. Since $A$ is of full rank, Eq. (40) has a unique solution as $\tilde{p} = A^{-1} \tilde{r}$. It is obvious that if $\tilde{p}_i \in [0, 1]$ for all $i$, one will directly obtain the optimal solution $p = A^{-1} \tilde{r}$. However, if there exist $\tilde{p}_i \notin [0, 1]$, this means the optimal solution doesn’t satisfy the constraints $p_i \in [0, 1]$. So the optimal solutions can only be present at the boundaries of $p_i \in [0, 1]$. Following the Lagrangian multiplier method similar to the proof of Theorem 2, the Karush-Kuhn-Tucker condition indicates that the optimal solution should be

$$\min_{i \prec j \prec k} D(\rho, \chi_{i,j,k}(\tilde{p})).$$  

(41)

It is shown that the current optimal scheme for $N = 4$ can be solved by Theorem 2. The proof is completed.

Up to now, we have entirely solved our optimal scheme with $N \leq 3$ and $N = 4$ with the full-rank matrix $A$. To proceed, we will have to first introduce a quite vital theorem 4, which is another cornerstone of our paper.

**Theorem 4.** Suppose $\{p_i, \rho_i\}_N$ to be the quantum state decomposition of a qubit state $\rho = \sum_{i=1}^{N} p_i \rho_i$ with $N \geq 4$. Let $R$ denote the rank of the $4 \times N$ matrix $A$ (obviously $R \leq 4$), then $R$ states as $\{q_j, \rho_j\}_R$ can always be found from $\{p_i, \rho_i\}_N$ to make another quantum state decomposition such that $\rho = \sum_{j=1}^{R} q_j \rho_j$ where $j = 1, 2, \cdots, R$ implies reordering the $R$ states and $R = 1$ means a quantum state as $\rho = \rho_1$.

Since the matrix $A$ is of rank $R$, one can always find $R$ linearly independent columns from $A$ and one additional column of $A$ to construct a $4 \times (R + 1)$ matrix denoted by $\hat{A}$. Here we’d like to use $\hat{A}$ to represent the $i$-th column of $\hat{A}$ with $i = 1, 2, \cdots, R + 1$. Additionally, we define $\hat{r}_o = [r_o; 1]$ for convenience. It is obvious that the $R + 1$ columns in $\hat{A}$ are linearly dependent, namely, there exist $k_i, i = 1, 2, \cdots, R + 1$ such that $\sum_{i=1}^{R+1} k_i A_i = 0$, which implies $\sum_{i=1}^{R+1} k_i = 0$ due to $A_{R+1} = 0$. In addition, Caratheodory theorem shows that $\hat{r}_o$ can be written as the convex mixing of the $R + 1$ columns of $\hat{A}$, i.e., $\hat{r}_o = \sum_{i=1}^{R+1} p_i A_i$ with $\sum_i p_i = 1$ and $\hat{p}_i \geq 0$. Thus
one can obtain
\[ \tilde{r}_\alpha = \sum_{i=1}^{R+1} p_i \tilde{A}_i - \alpha \sum_{i=1}^{R+1} k_i \tilde{A}_i = \sum_{i=1}^{R+1} p_i (1 - \alpha \frac{k_i}{p_i}) \tilde{A}_i. \]  

Let \( \alpha = \frac{p_{i'}}{k_i} = \min_{1 \leq i \leq R+1} \left\{ \frac{p_i}{k_i} | k_i > 0 \right\} \), we will find that
\[ 1 - \alpha \frac{k_i}{p_i} \left\{ \begin{array}{l} \geq 0 \quad i = i' \\ < 0 \quad i \neq i' \end{array} \right\} \] 
and \( \sum_i p_i (1 - \alpha \frac{k_i}{p_i}) = 1 \) which means that at most \( R \) columns of \( \tilde{A} \) are enough to convexly construct \( r_\alpha \). The proof is finished.

The importance of Theorem 4 is twofold. One is that if a density matrix can be written as the convex mixing of only \( S \) quantum states, Theorem 4 shows that \( R \leq 4 \) quantum states are enough to convexly prepare the given density matrix. The other is that the \( R \leq 4 \) quantum states aren’t so arbitrary that they can be exactly found from the previous \( N \geq 4 \) quantum states. In other words, if \( N \geq 4 \) quantum states in set \( S \) can optimally construct a given density matrix, one can select \( R \leq 4 \) from the \( N \) quantum states to construct the given density matrix with an equal optimization degree. This can also be given in the following rigorous way.

**Theorem 5.** For \( N \geq 4 \) with \( 4 \times N \) rank-\( R \) matrix \( A \), the optimal approximation is determined by
\[ \min_{i_1 < i_2 < \cdots < i_n} D(\rho, \chi_{i_1}, \chi_{i_2}, \cdots, \chi_{i_n} (\tilde{\rho})), i_\alpha = 1, 2, \cdots, N. \]

**Proof.** The proof of this theorem is straightforward. Suppose we can select \( N' \geq R \) quantum states from the set \( S \) to prepare the state denoted by \( \rho_o = \sum_{i=1}^{N'} \rho_i \) such that \( D(\rho, \rho_o) \) achieves the optimal distance. Theorem 4 indicates that one can always find \( R \) states from the selected \( N' \) quantum states to exactly prepare the state \( \rho_o \) with some proper weights. This implies that for \( N \geq 4 \), the convex mixing of only \( R \) states in \( S \) is enough to achieve the optimal distance. Therefore, we can directly consider all potential combinations of only \( R \) quantum states among the set \( S \). The minimal distance will give our expected optimal result, which is exactly what Theorem 5 says.

**Examples.** To further demonstrate the validity of our theorems and their applications, we will consider various randomly generated objective states and set \( S \) by comparing our analytical results with the numerical ones. For simplicity, we’d like to write the objective density matrix as \( \rho = \left( \begin{array}{cc} 1 - a & k \sqrt{a(1 - a)} e^{i \phi} \\ k \sqrt{a(1 - a)} e^{-i \phi} & a \end{array} \right) \) with \( k, a \in [0, 1] \) and \( \Phi \) denoting the phase, and the explicit forms of \( S = \{ \rho_1, \rho_2, \cdots, \rho_N \} \) in all the below examples are given in the Appendix A.

(i) \( N = 2 \). The random phase for the objective state \( \rho \) is given by \( \Phi = 1.3580 \pi \) with \( \{ k = 0.2, 0.4, 0.6, 0.8 \} \). The optimal distance denoted by \( D(\rho) \) versus \( a \in [0, 1] \) is plotted in Fig. 1 (a), which shows the perfect consistency between the numerical and the analytical results, and further supports our theorem 1.

(ii) \( N = 3 \). The objective state \( \rho \) is generated with a random phase \( \Phi = 0.4511 \pi \) and \( \{ a = 0.2, 0.4, 0.6, 0.8 \} \). The optimal distance \( D(\rho) \) versus \( k \in [0, 1] \) is plotted in Fig. 1 (b), which validates our theorem 2 based on the perfect consistency.

(iii) \( N = 4 \). The objective state \( \rho \) is generated by the randomly generated \( a = 0.7522 \) with \( \{ k = 0.2, 0.4, 0.6, 0.8 \} \). The optimal distance \( D(\rho) \) versus \( \Phi \in [0, 2\pi] \) is plotted in Fig. 1 (c). This indicates the perfect consistency with our theorem 3.

(iv) \( N = 4 \) with two pairs of orthonormal states. The objective state \( \rho \) is given by a random \( a = 0.3135 \) and \( \Phi = \frac{1}{2} \pi, \pi, \frac{1}{2} \pi, 2 \pi \). We set \( \{ \varphi_1, \varphi_2 \} = 0 \) and \( \{ \varphi_3, \varphi_4 \} = 0 \) which can be found in the Appendix B. The optimal distance \( D(\rho) \) versus \( k \in [0, 1] \) is plotted in Fig. 1 (d), which is perfectly consistent with our theorem 4.

(v) \( N = 5 \). The objective state \( \rho \) is established with \( k = 0.5625 \), \( \{ a = 0.2, 0.4, 0.6, 0.8 \} \) and the free \( \Phi \in [0, 2\pi] \). The optimal distance \( D(\rho) \) versus \( \Phi \) is plotted in Fig. 2 (a), which shows our theorem 4 and theorem 5 are valid.

(vi) \( N = 10 \). To further illustrate the application of our main results to large-scale cases. We consider the quantum state set \( S \), which includes ten states. The objective state \( \rho \) is determined by the random \( \Phi = \frac{1}{2} \pi, \pi, \frac{3}{2} \pi, 2 \pi \) and the free \( a \in [0, 1] \). The optimal distance \( D(\rho) \) versus \( a \) is plotted in Fig. 2 (b).

(vii) *The set S of the eigenstates of Pauli matrices.* Besides the above numerical tests, we give an analytic example. The pure-state set \( S \) is made up of the eigenstates of two Pauli matrices \( \sigma_x \) and \( \sigma_y \), i.e., \( \{ \varphi_{2 \pm} \} = (1, \pm 1)^T / \sqrt{2} \). In this case, one can find that the rank of matrix \( A \) is equal to 3, so based on our theorems, we only require three among the four quantum states to solve the optimal scheme.
If $\Lambda > 0$ and the optimal weights as tum states can be converted into the problem with not the Appendix B. about the various cases of the Pauli-distance is given in

Similar results can be found in [36]. The whole story formations the Pauli-distance is invariant under the state transfor-

D$ FIG. 2: (color online) The optimal distance $D(\rho)$ versus $\Phi$. The strictly analytical solutions correspond to the solid line and the numerical solutions are marked with “+”.

the Pauli-distance is invariant under the state transformations $\rho(a, k, \Phi) \rightarrow \rho(a, k, \Phi \pm n\pi/2)$ (with the integer $n$), it is enough only to consider $\Phi \in [0, \pi/2]$. If $\Lambda = r_{ox} + r_{oy} \leq 1$, one can calculate the optimal dis-

and the optimal weights as

$$p_{1+} = r_{ox}p_{1-} = 0,$$

$$p_{2-} = \frac{1}{2} [1 - \Lambda], p_{1+} = 1 - p_{1+} - p_{2-},$$

or

$$p_{2+} = r_{oy}p_{2-} = 0,$$

$$p_{1-} = \frac{1}{2} [1 - \Lambda], p_{1+} = 1 - p_{1+} - p_{2+};$$

If $\Lambda > 1$, the optimal distance is given by

$$D^2(\rho, \chi_{1,2,3,4} (\vec{p})) = r_{oz}^2 + \frac{1}{2} (r_{ox} + r_{oy} - 1)^2,$$

and the optimal weights as

$$p_{1+} = \frac{1}{2} [1 + r_{ox} - r_{oz}],$$

$$p_{2+} = 1 - p_{1+}, p_{1-} = p_{2-} = 0.$$

Notice the identities

$$r_{ox} = 2k\sqrt{a(1-a)} \cos \Phi,$$

$$r_{oy} = 2k\sqrt{a(1-a)} \sin \Phi,$$

$$r_{oz} = 1 - 2a.$$

Similar results can be found in [36]. The whole story about the various cases of the Pauli-distance is given in the Appendix B.

Conclusions and discussion.—To sum up, we have thoroughly solved the optimal approximation of a qubit state with the given quantum state set. The key points are that this type of problems is a convex optimization problem, and the optimal approximation with $N \geq 4$ quan-

solve the cases with not more than four quantum states and equivalently solve the whole question. We’d like to mention that an interesting link between the optimal approximation and the triple uncertainty relation was given in Ref. [37], where the state set with four pure states was also addressed. However, the four (or six) qubit pure states considered in Ref. [37] are two (or three) pairs of orthogonal qubit pure states restricted in real space. Our current work extends the given state set to include arbitrary number of qubit states and especially loosens the restriction not only from real to complex quantum states, but also from pure to mixed states.

Finally, we emphasize that the distance here is based on the trace norm of two states. Other distances of states should also be feasible and be worth studying. Besides, we only consider the optimal approxima-

Appendix A: The explicit forms of the set $S$ for examples

In example (i), the quantum state set $S$ includes two randomly generated quantum states whose Bloch vectors are

$$r_1 = (0.7888 \ 0.1788 \ -0.1182)^T,$$

$$r_2 = (0.4715 \ 0.4288 \ 0.5066)^T.$$  \hspace{1cm} (A1)

In example (ii), the quantum state set $S$ is given in Bloch representation as

$$r_1 = (-0.0347 \ 0.0178 \ 0.0088)^T,$$

$$r_2 = (0.3369 \ -0.7514 \ -0.2106)^T,$$

$$r_3 = (0.3784 \ 0.8012 \ -0.4636)^T.$$ \hspace{1cm} (A2)

The quantum state $r_3$ is a pure state.
The quantum states \( r \) are randomly generated quantum states which are with
\[
\begin{align*}
|\varphi_1\rangle &= \left( \begin{array}{c}
0.5951 - 0.1605i \\
-0.2363 + 0.001i
\end{array} \right), \\
|\varphi_2\rangle &= \left( \begin{array}{c}
0.2495 + 0.605i \\
0.9665 + 0.0028i
\end{array} \right), \\
|\varphi_3\rangle &= \left( \begin{array}{c}
0.5140 + 0.1652i \\
-0.4624 - 0.179i
\end{array} \right), \\
|\varphi_4\rangle &= \left( \begin{array}{c}
-0.3277 + 0.698i \\
0.6347 + 0.0374i
\end{array} \right).
\end{align*}
\] (A3)

Note that \( \langle \varphi_1 | \varphi_2 \rangle = 0 \) and \( \langle \varphi_3 | \varphi_4 \rangle = 0 \).

In example (iv), the quantum state set \( S \) includes five randomly generated quantum states which are
\[
\begin{align*}
|\rho_1\rangle &= \left( \begin{array}{c}
-0.4767 + 0.5882 - 0.6051i
\end{array} \right), \\
|\rho_2\rangle &= \left( \begin{array}{c}
0.3041 - 0.2655 + 0.1277i
\end{array} \right), \\
|\rho_3\rangle &= \left( \begin{array}{c}
0.0459 - 0.3519 + 0.0202i
\end{array} \right), \\
|\rho_4\rangle &= \left( \begin{array}{c}
0.7263 - 0.1260 - 0.6758i
\end{array} \right), \\
|\rho_5\rangle &= \left( \begin{array}{c}
-0.5631 - 0.5566 + 0.6108i
\end{array} \right).
\end{align*}
\] (A4)

The quantum states \( r_1 \) and \( r_5 \) are pure states.

In example (v), we consider the set \( S \) composed of 10 randomly generated quantum states which are listed as follows.
\[
\begin{align*}
|\rho_1\rangle &= \left( \begin{array}{c}
-0.0192 + 0.5339 + 0.4067i
\end{array} \right), \\
|\rho_2\rangle &= \left( \begin{array}{c}
-0.0299 + 0.0694 - 0.1474i
\end{array} \right), \\
|\rho_3\rangle &= \left( \begin{array}{c}
0.1865 - 0.2202 - 0.0863i
\end{array} \right), \\
|\rho_4\rangle &= \left( \begin{array}{c}
0.4860 - 0.3405 + 0.5005i
\end{array} \right), \\
|\rho_5\rangle &= \left( \begin{array}{c}
-0.4864 - 0.4754 + 0.4707i
\end{array} \right),
\end{align*}
\] (A5)
and
\[
\begin{align*}
|\rho_6\rangle &= \left( \begin{array}{c}
-0.5738 - 0.0250 + 0.5583i
\end{array} \right), \\
|\rho_7\rangle &= \left( \begin{array}{c}
-0.0071 + 0.0058 - 0.0298i
\end{array} \right), \\
|\rho_8\rangle &= \left( \begin{array}{c}
-0.5357 - 0.7338 + 0.4177i
\end{array} \right), \\
|\rho_9\rangle &= \left( \begin{array}{c}
-0.9142 + 0.8293 - 0.8847i
\end{array} \right), \\
|\rho_{10}\rangle &= \left( \begin{array}{c}
0.4888 + 0.8306 + 0.2670i
\end{array} \right).
\end{align*}
\] (A6)

The quantum states \( r_8, r_9 \) and \( r_{10} \) are pure states.

### Appendix B: Explicit calculation of the cases of Pauli matrices

Let \( |z\rangle_s = \{|0\rangle_s, |1\rangle_s\} \), \( |x\rangle_s = \{\frac{1}{\sqrt{2}}(|0\rangle_s \pm |1\rangle_s)\} \) and \( |y\rangle_s = \{\frac{1}{\sqrt{2}}(|0\rangle_s \pm i|1\rangle_s)\} \) be the eigenstates of the Pauli matrices \( \sigma_z, \sigma_x \) and \( \sigma_y \), respectively. \( s = \pm 1 \) are the eigenvalues.

Since the Pauli-distance is invariant under the state transformations \( \rho(a, k, \Phi) \rightarrow \rho(1 - a, k, \Phi) \) and \( \rho(a, k, \Phi) \rightarrow \rho(a, k, \Phi \pm n\pi/2) \) (with the integer \( n \)), it is enough only to consider \( a \in [0, 1/2] \) and \( \Phi \in [0, \pi/2] \). We have
\[
\begin{align*}
r_{ox} &= 2k\sqrt{a(1-a)} \cos \Phi, \\
r_{oy} &= 2k\sqrt{a(1-a)} \sin \Phi, \\
r_{oz} &= 1 - 2a.
\end{align*}
\] (B1)

We study our scheme step by step from \( N = 3, N = 4 \) and \( N = 6 \).

For \( N = 3 \), we choose three of the six quantum states to solve the convex optimization problem. This problem can be divided into the following four cases.

**Case 1.** The three selected quantum states are \( |\alpha_1\rangle, |\alpha_2\rangle, |\alpha_3\rangle \) with \( \alpha_1 \neq \alpha_2 \neq \alpha_3 \) and \( |\alpha_4\rangle, |\alpha_5\rangle, |\alpha_6\rangle \) with \( \alpha_4 \neq \alpha_5 \neq \alpha_6 \). If \( s_3 = 1 \) and \( r_{ox} + r_{oz} \leq 1 \), one can calculate the optimal distance as
\[
D(\rho, \chi_{1,2,3} (\tilde{p})) = r_{ox} + r_{oz},
\] (B2)
and the optimal weights as
\[
\begin{align*}
p_1 &= 1 - p_2 - p_3, \\
p_2 &= \frac{1}{2} (1 - r_{ox} - r_{oz}), \\
p_3 &= r_{oz}.
\end{align*}
\] (B3)

If \( s_3 = 1 \) and \( r_{ox} + r_{oz} > 1 \), the optimal distance is given by
\[
D^2(\rho, \chi_{1,3} (\tilde{p})) = r_{ox}^2 + \frac{1}{2} (r_{ox} + r_{oz} - 1)^2,
\] (B4)
and the optimal weights are given by
\[
\begin{align*}
p_1 &= \frac{1}{2} (1 + r_{ox} - r_{oz}), \\
p_3 &= 1 - p_1, p_2 = 0,
\end{align*}
\] (B5)

If \( s_3 = -1 \), the optimal distance is given by
\[
D^2(\rho, \chi_{1,2} (\tilde{p})) = r_{ox}^2 + r_{oz}^2,
\] (B6)
and the optimal weights are
\[
\begin{align*}
p_1 &= \frac{1}{2} (1 + r_{ox}), \\
p_2 &= 1 - p_1, p_3 = 0.
\end{align*}
\] (B7)

**Proof.** The mutually orthogonal \( |\varphi_1\rangle \) and \( |\varphi_2\rangle \) mean that \( r_{10}^T r_2 = -1 \). From \( r_1^T r_3 = r_2^T r_3 = 0 \), we can get
\[
\begin{align*}
\tilde{R}_{13} &= \tilde{R}_{23} = -2, \\
\tilde{R}_{12} &= 0, d = 4.
\end{align*}
\] (B8)
Substituting these parameters into Theorem 2, one will obtain the pseudo-probabilities for the problem as

\[ \hat{p}_1 = 1 - \hat{p}_2 - \hat{p}_3, \]
\[ \hat{p}_2 = \frac{1}{2} \left( 1 - r_{oa} - r_{oa'}, s_3 \right), \]
\[ \hat{p}_3 = r_{oa'} s_3. \] \hspace{1cm} (B9)

The necessary and sufficient condition of restriction \( \hat{p}_i \geq 0 \) holds for \( i = 1, 2, 3 \) is

\[ r_{oa} + r_{oa'} \leq 1, s_3 = 1. \] \hspace{1cm} (B10)

If \( s_3 = 1 \) and \( r_{oa} + r_{oa'} > 1 \), the optimal distance is given by

\[ \min_{i < j} D(\rho, \chi_{i,j}(\tilde{p})), i, j, k = 1, 2, 3. \] \hspace{1cm} (B11)

By using Theorem 1, we can get

\[ D^2(\rho, \chi_{1,3}(\tilde{p})) = r^2_{oa''} + \frac{1}{2} \left( r_{oa} + r_{oa'} - 1 \right)^2, \]
\[ D^2(\rho, \chi_{1,2}(\tilde{p})) = r^2_{oa'} + r^2_{oa''}, \] \hspace{1cm} (B12)

and

\[ D^2(\rho, \chi_{2,3}(\tilde{p})) = \min \{ D^2(\rho, \chi_{1,2}(\tilde{p})), D^2(\rho, \chi_{3}(\tilde{p})) \} = \min \{ 1 + r_o^T r_o + 2r_{oa} + 1 + r_o^T r_o - 2r_{oa} \} = 1 + \frac{r_o^T r_o}{2} \geq 0. \] \hspace{1cm} (B13)

Next we compare the three quantities in Eq. (B12) and Eq. (B13). We have

\[ D^2(\rho, \chi_{1,3}(\tilde{p})) - D^2(\rho, \chi_{1,2}(\tilde{p})) = \frac{1}{2} \left( r_{oa} + r_{oa'} - 1 \right)^2 - r^2_{oa'}, \]
\[ = \frac{1}{2} \left( r_{oa} + r_{oa'} - 1 + \sqrt{2}r_{oa} \right) \left( r_{oa} + r_{oa'} - 1 - \sqrt{2}r_{oa} \right) \leq 0. \] \hspace{1cm} (B14)

and

\[ D^2(\rho, \chi_{1,3}(\tilde{p})) - D^2(\rho, \chi_{2,3}(\tilde{p})) = \frac{1}{2} \left( r_{oa} + r_{oa'} - 1 \right)^2 - 1 - r_o^T r_o + 2r_{oa}, \]
\[ = - \frac{1}{2} \left( r_{oa} + r_{oa'} + 1 \right)^2 < 0. \] \hspace{1cm} (B15)

So \( \min_{i < j} D(\rho, \chi_{i,j}(\tilde{p})) \) can be realized by the quantum state set \( \{ |\varphi_1\rangle, |\varphi_2\rangle \} \), and the optimal distance and weights can be calculated by Eqs. (B14) and (B15), respectively.

If \( s_3 = -1 \), we have

\[ D^2(\rho, \chi_{1,2}(\tilde{p})) = r^2_{oa'} + r^2_{oa''}, \]
\[ D^2(\rho, \chi_{2,3}(\tilde{p})) = r^2_{oa''} + \frac{1}{2} \left( r_{oa} + r_{oa'} + 1 \right)^2 \] \hspace{1cm} (B16)

and

\[ D^2(\rho, \chi_{1,2}(\tilde{p})) - D^2(\rho, \chi_{2,3}(\tilde{p})) = \frac{1}{2} \left( \left( r_{oa} + r_{oa'} + 1 \right)^2 \right) - \frac{1}{2} \left( r_{oa} + r_{oa'} + 1 \right)^2 \]
\[ = \frac{1}{2} \left( \left( \sqrt{2}r_{oa'} + r_{oa} + r_{oa'} + 1 \right)^2 \left( \sqrt{2}r_{oa'} - r_{oa} - r_{oa'} - 1 \right) \right) < 0. \] \hspace{1cm} (B17)

If \( s_3 = -1 \) and \( r_{oa} + r_{oa'} \leq 1 \), we have

\[ D^2(\rho, \chi_{1,3}(\tilde{p})) = r^2_{oa''} + \frac{1}{2} \left( r_{oa} - r_{oa'} - 1 \right)^2, \] \hspace{1cm} (B18)

and

\[ D^2(\rho, \chi_{1,2}(\tilde{p})) - D^2(\rho, \chi_{1,3}(\tilde{p})) \]
\[ = \frac{1}{2} \left( \left( \sqrt{2}r_{oa'} - r_{oa} + r_{oa'} + 1 \right)^2 \left( \sqrt{2}r_{oa'} - r_{oa} + r_{oa'} + 1 \right) \right) < 0. \] \hspace{1cm} (B19)

If \( s_3 = -1 \) and \( r_{oa} + r_{oa'} > 1 \), we have

\[ D^2(\rho, \chi_{1,3}(\tilde{p})) = \min \{ D^2(\rho, \chi_{1,2}(\tilde{p})), D^2(\rho, \chi_{1,3}(\tilde{p})) \} = \min \{ 1 + r_o^T r_o, r_o^T r_o - 2r_{oa}, 1 + r_o^T r_o + 2r_{oa} \} = 1 + r_o^T r_o - 2r_{oa}. \] \hspace{1cm} (B20)

and

\[ D^2(\rho, \chi_{1,2}(\tilde{p})) - D^2(\rho, \chi_{1,3}(\tilde{p})) = r_o^T r_o - 2r_{oa}, \]
\[ = - (1 - r_{oa})^2 < 0. \] \hspace{1cm} (B21)

So \( \min_{i < j} D(\rho, \chi_{i,j}(\tilde{p})) \) can be realized by the quantum state set \( \{ |\varphi_1\rangle, |\varphi_2\rangle \} \), and the optimal distance and weights can be calculated by Eqs. (B16) and (B17), respectively. The proof is completed.

**Case 2.** If \( |\varphi_1\rangle = |x\rangle_{s_x}, |\varphi_2\rangle = |y\rangle_{s_y} \) and \( |\varphi_3\rangle = |z\rangle_{s_z} \), the pseudo-probabilities for the problem can be first given by

\[ \tilde{p}_x = \frac{1}{3} \left( 1 + 2r_{ox}s_x - r_{oy}s_y - r_{oz}s_z \right), \]
\[ \tilde{p}_y = \frac{1}{3} \left( 1 + 2r_{oy}s_y - r_{ox}s_x - r_{oz}s_z \right), \]
\[ \tilde{p}_z = 1 - \tilde{p}_x - \tilde{p}_y. \] \hspace{1cm} (B22)

If \( \tilde{p}_i \geq 0 \) holds for \( i = x, y, z \), the optimal weights \( p_i = \tilde{p}_i \), and the optimal distance are given by

\[ D(\rho, \chi_{x,y,z}(\tilde{p})) = \frac{\sqrt{3}}{3} \left( 1 - 2r_{ox}s_x - r_{oy}s_y - r_{oz}s_z \right). \] \hspace{1cm} (B23)

If \( s_x = s_y = s_z = 0 \) with \( \alpha \neq \alpha' \neq \alpha'' \) and \( \alpha, \alpha', \alpha'' = x, y, z \), the optimal distance is given by

\[ D^2(\rho, \chi_{\alpha',\alpha''}(\tilde{p})) = r^2_{oa} + \frac{1}{2} \left( r_{oa'} + r_{oa''} - s_z \right)^2, \] \hspace{1cm} (B24)
and the optimal weights are given by
\[ p_{a'} = \frac{1}{2} \left( 1 + s_x (r_{oa'} - r_{oa''}) \right), \]
\[ p_{a''} = 1 - p_{a'}, p_a = 0. \]  \hspace{1cm} (B25)

If \( s_a = 1, s_{a'} = s_{a''} = -1, p_{a'} < 0 \) and \( r_{oa} + r_{oa''} \leq 1 \),
the optimal distance is given by
\[ D(\rho, \chi_{a,a''} (\tilde{p})) = r_{oa''}^2 + \frac{1}{2} (r_{oa} - r_{oa''} - 1)^2, \]  \hspace{1cm} (B26)

and the optimal weights are
\[ p_a = \frac{1}{2} (1 + r_{oa} + r_{oa''}), \]
\[ p_{a''} = 1 - p_{a'}, p_{a'} = 0. \]  \hspace{1cm} (B27)

If \( s_a = 1, s_{a'} = s_{a''} = -1, p_{a'} < 0 \) and \( r_{oa} + r_{oa''} > 1 \),
the optimal distance is given by
\[ D(\rho, \chi_a (\tilde{p})) = 1 + r_{oa}^2, \]  \hspace{1cm} (B28)

and the optimal weights are
\[ p_a = 1, p_{a'} = p_{a''} = 0. \]  \hspace{1cm} (B29)

If \( s_a = s_{a'} = 1, s_{a''} = -1 \) and \( \tilde{p}_{a''} < 0 \),
the optimal distance is given by
\[ D(\rho, \chi_{a,a'} (\tilde{p})) = r_{oa''}^2 + \frac{1}{2} (r_{oa} + r_{oa'} - 1)^2, \]  \hspace{1cm} (B30)

and the optimal weights are
\[ p_a = \frac{1}{2} (1 + r_{oa} - r_{oa'}), \]
\[ p_{a'} = 1 - p_{a''}, p_{a''} = 0. \]  \hspace{1cm} (B31)

**Proof.** For these three special quantum states, we have
\[ r_i^T r_j = 0, \tilde{R}_{ij} = -1, d = 3, \]  \hspace{1cm} (B32)

with \( i, j = x, y, z \). Substitute these parameters into Theorem 2, one will obtain
\[
\begin{align*}
\tilde{p}_x &= \frac{1}{3} (1 + 2r_{ox} s_x - r_{oy} s_y - r_{oz} s_z), \\
\tilde{p}_y &= \frac{1}{3} (1 + 2r_{oy} s_y - r_{ox} s_x - r_{oz} s_z), \\
\tilde{p}_z &= 1 - \tilde{p}_x - \tilde{p}_y.
\end{align*}
\]  \hspace{1cm} (B33)

If \( \tilde{p}_i \geq 0 \) holds for \( i = x, y, z \), the optimal weights are given by \( p_i = \tilde{p}_i \) and the optimal distance
\[ D(\rho, \chi_{x,y,z} (\tilde{p})) = \frac{\sqrt{3}}{3} (1 - 2r_{ox} s_x - r_{oy} s_y - r_{oz} s_z). \]  \hspace{1cm} (B34)

Otherwise, we consider the following three cases.

Case 2.1. \( s_x = s_y = s_z \). If \( \tilde{p}_x < 0 \) with \( \alpha \neq \alpha' \neq \alpha'' |a, \alpha', \alpha'' = x, y, z, \) the optimal distance is given by
\[ \min_{i<j} D(\rho, \chi_{i,j} (\tilde{p})), i, j = x, y, z. \]  \hspace{1cm} (B35)

From \( \tilde{p}_a < 0 \), we can get
\[ 1 + s_x (2r_{oa} - r_{oa'} - r_{oa''}) < 0. \]

Using Theorem 1, we can get
\[ D^2(\rho, \chi_{a,a'} (\tilde{p})) = r_{oa''}^2 + \frac{1}{2} (r_{oa} + r_{oa'} - s_x)^2. \]  \hspace{1cm} (B36)

Next we compare the above three combinations. We have
\[
\begin{align*}
D^2(\rho, \chi_{a,a'} (\tilde{p})) - D^2(\rho, \chi_{a,a''} (\tilde{p})) &= r_{oa''}^2 + \frac{1}{2} (r_{oa} + r_{oa'} - s_x)^2 - \frac{1}{2} (r_{oa} + r_{oa''} - s_x)^2 \\
&= \frac{1}{2} (r_{oa''} - r_{oa}) (2r_{oa''} - 2s_x - r_{oa} - r_{oa''}) < 0,
\end{align*}
\]  \hspace{1cm} (B37)

and
\[
\begin{align*}
D^2(\rho, \chi_{a,a''} (\tilde{p})) - D^2(\rho, \chi_{a,a'} (\tilde{p})) &= r_{oa''}^2 + \frac{1}{2} (r_{oa} + r_{oa''} - s_x)^2 - \frac{1}{2} (r_{oa} + r_{oa'} - s_x)^2 \\
&= \frac{1}{2} (r_{oa''} - r_{oa}) (2r_{oa''} - 2s_x - r_{oa} - r_{oa''}) < 0.
\end{align*}
\]  \hspace{1cm} (B38)

So \( \min_{i<j} D(\rho, \chi_{i,j} (\tilde{p})) \) can be realized by the quantum state set \( \{\alpha', \alpha''\} \), and the optimal distance and the weights can be calculated as Eqs. \[[24] \text{ and } [25], \] respectively.

Case 2.2. \( s_a = 1, s_{a'} = s_{a''} = -1 \). We can find that \( \tilde{p}_a = \frac{1}{3} (1 + 2r_{oa} + r_{oa'} + r_{oa''}) > 0 \). If \( \tilde{p}_a < 0 \) with \( \alpha \neq \alpha' \neq \alpha'' |a, \alpha', \alpha'' = x, y, z, \) the optimal distance is given by
\[ \min_{i<j} D(\rho, \chi_{i,j} (\tilde{p})), i, j = x, y, z. \]  \hspace{1cm} (B39)

From \( \tilde{p}_a < 0 \), we can get
\[ 1 + r_{oa''} - 2r_{oa'} - r_{oa} < 0. \]  \hspace{1cm} (B40)

By using Theorem 1, we can get
\[ D^2(\rho, \chi_{a,a''} (\tilde{p})) = r_{oa''}^2 + \frac{1}{2} (r_{oa' + r_{oa''} + 1})^2. \]  \hspace{1cm} (B41)

Case 2.2.1. \( r_{oa} + r_{oa''} \leq 1 \). Based on Theorem 1, we can get
\[ D^2(\rho, \chi_{a,a''} (\tilde{p})) = r_{oa''}^2 + \frac{1}{2} (r_{oa} - r_{oa''} - 1)^2. \]  \hspace{1cm} (B42)

Thus we have
\[
\begin{align*}
D^2(\rho, \chi_{a,a''} (\tilde{p})) - D^2(\rho, \chi_{a,a'} (\tilde{p})) &= \frac{1}{2} (r_{oa''} - r_{oa'}) (2 - 2r_{oa} - r_{oa'} - r_{oa''}) \\
&< 0.
\end{align*}
\]  \hspace{1cm} (B43)
If \( r_{ao} + r_{ao'} \leq 1 \), we have

\[
D^2(\rho, \chi_{\alpha,\alpha'} (\vec{p})) = r_{ao}^2 + \frac{1}{2} (r_{ao} - r_{ao'})^2, \tag{B44}
\]

and

\[
D^2(\rho, \chi_{\alpha,\alpha''} (\vec{p})) - D^2(\rho, \chi_{\alpha,\alpha'} (\vec{p})) = \frac{1}{2} (r_{ao'} - r_{ao}) (2 - 2r_{ao} - r_{ao'} - r_{ao''}) < 0. \tag{B45}
\]

If \( r_{ao} + r_{ao'} > 1 \), we have

\[
D^2(\rho, \chi_{\alpha,\alpha'} (\vec{p})) = D^2(\rho, \chi_{\alpha} (\vec{p})), \tag{B46}
\]

and

\[
D^2(\rho, \chi_{\alpha,\alpha''} (\vec{p})) < D^2(\rho, \chi_{\alpha} (\vec{p})). \tag{B47}
\]

So \( \min_{i<j} D(\rho, \chi_{ij} (\vec{p})) \) can be realized by the quantum state set \( \{ |\alpha\rangle, |\alpha''\rangle \} \), and the optimal distance and the weights can be calculated as Eqs. (B26) and (B27), respectively.

Case 2.2.2.- \( r_{ao} + r_{ao'} > 1 \). Combined with Eq. (B40), we can get \( r_{ao} + r_{ao'} > 1 \) and \( r_{ao'} > r_{ao''} \). By using Theorem 1, we can get

\[
D^2(\rho, \chi_{\alpha,\alpha'} (\vec{p})) = D^2(\rho, \chi_{\alpha,\alpha''} (\vec{p})) = D^2(\rho, \chi_{\alpha} (\vec{p})) = 1 + r_{ao}^2 r_o - 2r_{ao}, \tag{B48}
\]

and

\[
D^2(\rho, \chi_{\alpha,\alpha',\alpha''} (\vec{p})) = D^2(\rho, \chi_{\alpha,\alpha''} (\vec{p})) = \frac{1}{2} \left[ 4(1 - r_{ao} - r_{ao'}) + (r_{ao'} - r_{ao''})(2 + r_{ao'} - r_{ao''}) - 3 \right] < 0. \tag{B49}
\]

So \( \min_{i<j} D(\rho, \chi_{ij} (\vec{p})) \) can be realized by the quantum state set \( \{ |\alpha\rangle \} \). The optimal distance and the weights can be calculated as Eqs. (B28) and (B29), respectively.

Case 2.3.- \( s_{\alpha} = s_{\alpha'} = 1, s_{\alpha''} = 1 \). We can find that \( \bar{p}_{\alpha} = \frac{1}{4} (1 + 2r_{ao} + r_{ao'} - r_{ao''}) > 0 \) and \( \bar{p}_{\alpha'} = \frac{1}{4} (1 + 2r_{ao'} + r_{ao} - r_{ao''}) > 0 \). If \( \bar{p}_{\alpha'} < 0 \), the optimal distance is given by

\[
\min_{i<j} D(\rho, \chi_{ij} (\vec{p})), i, j = x, y, z. \tag{B50}
\]

By using Theorem 1, we can get

\[
D^2(\rho, \chi_{\alpha,\alpha'} (\vec{p})) = r_{ao'}^2 + \frac{1}{2} (r_{ao} - r_{ao'})^2. \tag{B51}
\]

If \( r_{ao} + r_{ao'} \leq 1 \), we have

\[
D^2(\rho, \chi_{\alpha,\alpha''} (\vec{p})) = r_{ao'}^2 + \frac{1}{2} (r_{ao} - r_{ao''} - 1)^2, \tag{B52}
\]

and

\[
D(\rho, \chi_{\alpha,\alpha'} (\vec{p})) - D(\rho, \chi_{\alpha,\alpha''} (\vec{p})) = \frac{1}{2} (r_{ao'} + r_{ao''}) (r_{ao''} + 2r_{ao} - 2 - r_{ao'}) < 0. \tag{B53}
\]

If \( r_{ao} + r_{ao'} > 1 \), we have

\[
D(\rho, \chi_{\alpha,\alpha'} (\vec{p})) = D(\rho, \chi_{\alpha} (\vec{p})) = 1 + r_{ao}^T r_o - 2r_{ao}, \tag{B54}
\]

and

\[
D(\rho, \chi_{\alpha,\alpha'} (\vec{p})) \leq D(\rho, \chi_{\alpha} (\vec{p})). \tag{B55}
\]

Through a similar process from Eq. (B52) to Eq. (B55), we can get

\[
D(\rho, \chi_{\alpha,\alpha'} (\vec{p})) \leq D(\rho, \chi_{\alpha,\alpha''} (\vec{p})). \tag{B56}
\]

To sum up, we can conclude that if \( s_{\alpha} = s_{\alpha'} = 1, s_{\alpha''} = 1 \), then \( \min_{i<j} D(\rho, \chi_{ij} (\vec{p})) \) can be realized by the quantum state set \( \{ |\alpha\rangle, |\alpha'\rangle \} \). The optimal distance and the weights can be calculated as Eqs. (B30) and (B31), respectively. The proof is completed.

For \( N = 4 \), we choose four of the six quantum states to solve the convex optimization problem.

Case 3.- We set \( |\varphi_{1\pm}\rangle = |\alpha\rangle_{\pm} \) and \( |\varphi_{2\pm}\rangle = |\alpha'\rangle_{\pm} \) with \( \{ \alpha \neq \alpha' \neq \alpha'' | \alpha, \alpha', \alpha'' = x, y, z \} \). If \( r_{ao} + r_{ao'} \leq 1 \), one can calculate the optimal distance as

\[
D(\rho, \chi_{1,2,3} (\vec{p})) = r_{ao''}, \tag{B57}
\]

and the optimal weights as

\[
\begin{align*}
p_{1+} &= r_{ao}, p_{1-} = 0, \\
p_{2-} &= \frac{1}{2} (1 - r_{ao'} - r_{ao}), \\
p_{2+} &= 1 - p_{1+} - p_{2-}. \tag{B58}
\end{align*}
\]

or

\[
\begin{align*}
p_{2+} &= r_{ao'}, p_{2-} = 0, \\
p_{1-} &= \frac{1}{2} (1 - r_{ao} - r_{ao'}), \\
p_{1+} &= 1 - p_{1-} - p_{2+}. \tag{B59}
\end{align*}
\]

If \( r_{ao} + r_{ao'} > 1 \), the optimal distance is given by

\[
D^2(\rho, \chi_{1,2} (\vec{p})) = r_{ao''}^2 + \frac{1}{2} (r_{ao'} + r_{ao''} - 1)^2, \tag{B60}
\]

and the optimal weights are given by

\[
\begin{align*}
p_{1+} &= \frac{1}{2} (1 + r_{ao} - r_{ao'}), \\
p_{2+} &= 1 - p_{1+}, p_{1-} = p_{2-} = 0. \tag{B61}
\end{align*}
\]

Proof. If \( |\varphi_{1\pm}\rangle = |\alpha\rangle_{\pm} \) and \( |\varphi_{2\pm}\rangle = |\alpha'\rangle_{\pm} \) with \( \{ \alpha \neq \alpha' \neq \alpha'' | \alpha, \alpha', \alpha'' = x, y, z \} \), the rank of matrix A.
is equal to 3. According to Theorem 4, the optimal distance is given by
\[
\min_{i<j<k} D(\rho, \chi_{i,j,k}(\bar{p})), i, j, k = 1, 2, 3, 4. \tag{B62}
\]

According to Case 1, if we choose three quantum states from \{\{\varphi_{1\pm}\}, \{\varphi_{2\pm}\}\}, we can only choose \{\{\varphi_{1+}\}, \{\varphi_{2\pm}\}\} and \{\{\varphi_{1\pm}\}, \{\varphi_{2\pm}\}\}. And the corresponding probabilities are Eqs. (B58) and (B59). The necessary and sufficient condition of restriction \(\tilde{p}_i \geq 0\) holds for \(i = 1, 2, 3\) is
\[
\tilde{r}_{o\alpha} + \tilde{r}_{o\alpha'} \leq 1. \tag{B63}
\]

If \(r_{o\alpha} + r_{o\alpha'} > 1\), the optimal distance is given by
\[
\min_{i<j} D(\rho, \chi_{i,j}(\bar{p})), i, j, k = 1, 2, 3, 4. \tag{B64}
\]

According to Case 1, we can find \(\min_{i<j} D(\rho, \chi_{i,j}(\bar{p}))\) can be realized by the quantum state set \{\{\varphi_{1\pm}\}, \{\varphi_{2\pm}\}\}. And the optimal distance and weights can be calculated as Eqs. (B60) and (B61), respectively. The proof is completed.

Case 4.- We set \(\vert \varphi_1 \rangle = \vert \alpha \rangle_1\), \(\vert \varphi_2 \rangle = \vert \alpha \rangle_2\), \(\vert \varphi_3 \rangle = \vert \beta \rangle_3\), \(\vert \varphi_4 \rangle = \vert \gamma \rangle_4\) with \(\alpha \neq \alpha' \neq \alpha''\) and \(\beta \neq \alpha', \alpha'', \beta' = x, y, z\). If \(s_3 = 1, s_4 = 1\), \(r_{ox} + r_{oy} + r_{oz} \leq 1\), the objective state \(\rho\) can be exactly written as the convex sum of the 4 pure states. And the corresponding probabilities are given by
\[
\begin{align*}
\tilde{p}_1 &= \frac{1}{2} (1 + r_{ox} - r_{o\alpha'} - r_{o\alpha''}) \\
\tilde{p}_2 &= \frac{1}{2} (1 - r_{ox} - r_{o\alpha'} - r_{o\alpha''}) \\
\tilde{p}_3 &= r_{o\alpha'}, \tilde{p}_4 = r_{o\alpha''}.
\end{align*} \tag{B66}
\]

Otherwise, the optimal approximation is solved based on Case 2 as
\[
\min_{i<j<k} D(\rho, \chi_{i,j,k}(\bar{p})), i, j, k = 1, 2, 3, 4. \tag{B67}
\]

Proof. The rank of matrix \(A\) is equal to 4. For Pauli matrix, we have
\[
\begin{align*}
\bar{r}_{\pm} &= (\pm 1~0~0)^T, \\
\bar{r}_{\pm} &= (0~\pm 1~0)^T, \\
\bar{r}_{\pm} &= (0~0~\pm 1)^T.
\end{align*} \tag{B68}
\]
Substituting these parameters into Theorem 3, one will obtain \(A\). For example, if \(\vert \varphi_1 \rangle = \vert x \rangle_1, \vert \varphi_2 \rangle = \vert x \rangle_1, \vert \varphi_3 \rangle = \vert y \rangle_1\) and \(\vert \varphi_4 \rangle = \vert z \rangle_1\), we have
\[
A = \begin{pmatrix}
1 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & -1 \\
1 & 1 & 1 & 1
\end{pmatrix}, \tag{B69}
\]
and
\[
A^{-1} = \frac{1}{2} \begin{pmatrix}
1 & -1 & 1 & 1 \\
-1 & -1 & 1 & 1 \\
0 & 2 & 0 & 0 \\
0 & 0 & -2 & 0
\end{pmatrix}. \tag{B70}
\]
By
\[
\tilde{p} = A^{-1} \tilde{r} \tag{B71}
\]
in Theorem 3, we can get
\[
\begin{align*}
\tilde{p}_1 &= \frac{1}{2} (1 + r_{ox} - r_{o\alpha', s_3} - r_{o\alpha'', s_4}) \\
\tilde{p}_2 &= \frac{1}{2} (1 - r_{ox} - r_{o\alpha', s_3} - r_{o\alpha'', s_4}) \\
\tilde{p}_3 &= r_{o\alpha', s_3}, \tilde{p}_4 = r_{o\alpha'', s_4}.
\end{align*} \tag{B72}
\]
The necessary and sufficient condition of restriction \(\tilde{p}_i \geq 0\) holds for \(i = 1, 2, 3, 4\) is
\[
\begin{align*}
s_3 &= 1, s_4 = 1, \\
r_{ox} + r_{oy} + r_{oz} &\leq 1. \tag{B73}
\end{align*}
\]
Otherwise, the optimal approximation is solved based on Case 2 as
\[
\min_{i<j<k} D(\rho, \chi_{i,j,k}(\bar{p})), i, j, k = 1, 2, 3, 4. \tag{B74}
\]

The proof is completed.

For \(N = 6\), we choose all six quantum states \{\{\vert x \rangle_s, \vert y \rangle_s, \vert z \rangle_s\} | s = \pm 1\} to solve the convex optimization problem. According to theorem 5, the problem is equivalent to selecting four most suitable eigenstates from six eigenstates to find the best. The optimal distance is given by
\[
\begin{align*}
\min_{i<j<k<l} D(\rho, \chi_{i,j,k,l}(\bar{p})), i, j, k, l = 1, 2, 3, 4, 5, 6. \tag{B75}
\end{align*}
\]
which as well as the corresponding weights can be solved by Case 3 and Case 4.

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