A Quantum Observation Scheme Can Universally Identify Causalities from Correlations

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It has long been recognized as a difficult problem to determine whether the observed statistical correlation between two classical variables arise from causality or common causes. Recent research has shown that in quantum theoretical framework, the mechanisms of entanglement and quantum coherence provide an advantage in tackling this problem. In some particular cases, quantum common causes and quantum causality can be effectively distinguished using observations only. However, these solutions do not apply to all cases. There still exist enormous cases in which quantum common causes and quantum causality can not be distinguished. In this paper, along the line of considering unitary transformation as causality in the quantum world, we formally show quantum common causes and quantum causality are universally separable. Based on the analysis, we further provide a general method to discriminate the two.

I. INTRODUCTION

Common causes and causality are two building blocks in the Reichenbach’s principle of casual explanation [1]. The principle asserts that if two observed variables are found to be statistically correlated, it could be that the early variable directly causes the later one, i.e., the causality case, or both share a common cause, i.e., a correlation between them. In this paper, we focus on identifying the causality from the correlations in the quantum world using only experimental observations.

Despite the central role of causal explanations in science, how to discriminate causality from correlations is still a hard issue. In classic cases, it is only recently that a rigorous framework for causal inferring has been developed [2]. Its core ingredient is the possibility of external interventions on the early variable. However, in many scenarios, interventionist schemes are often impractical for the technical or ethical reasons.

In quantum cases, Bell theorem rules out the classical common cause explanation of the causal models that obeys a Bell inequality [3]. To make causal model be compatible with quantum mechanism, a considerable effort has been recently devoted, including applying the classical causal model by introducing hidden and fine tuned mechanisms [4], or alternatively transferring classical causal modeling tools to the quantum domain [5–10], then leading to a reformulation of quantum causal models [11–13]. Causal structures are usually represented as directed acyclic graphs in these methods and the established quantum version of Reichenbach’s principle allows one to perform Bayesian inference to analyze the causal structures.

Different from these methods, our work mainly motivated by Ref. [14, 15] is based on the frequentist inference, using the frequency of the particular events, i.e., the statistic, to identify the existence of common cause or causality. In Ref. [14], Reid et al. proposed the statistic C for the discrimination problem, where quantum causality and quantum common causes are represented as Pauli matrices and Bell states respectively. In Ref. [15], Hu et al. generalized the quantum common cases and quantum causality as general entanglement states and some unitary matrix in U(2) respectively and substituted C with a vector-valued function P. It is showed that in some particular causal scenarios, one can utilize P as well as C to distinguish quantum causality from quantum common causes by using experimental observation only. However, in the overlapping area between the statistic P of quantum common causes and that of quantum causality, they are still inseparable (see Fig. 1).

In this paper, we formally show that quantum common causes and quantum causality can be separable universally even though the value of P is initially in the overlapping area. We make this conclusion on the temporally ordered two qubits with the same setup as in Ref. [15]. The key idea behind the result is the same specified unitary transformation applied to the observables of the two qubits can make the statistic P change differently in terms of whether there exists a direct causal connection between them or there exists a common cause acting on them.

We first analyze the general representation forms of possible quantum common causes and possible quantum direct causes and discuss the changes of the value of P when unitary operators are applied on the observables. Second, four groups of unitary operators are carefully designed. We prove that in the causality case, there is
at least one group of unitary operations by which the value of $\mathbf{P}$ can be transferred to a fixed location; but in the common cause case, all unitary operations in these groups can not transfer the value of $\mathbf{P}$ to the same location except that $\mathbf{P}$ is initially in a particular measure zero area. Furthermore, we give a solution for the case that $\mathbf{P}$ is in the measure zero area. Third, based on the analysis, a new method is proposed to universally distinguish quantum common causes and quantum causality for all possible cases in question. Simulation experiments verify our theoretical results.

II. CONDUCT UNITARY OPERATIONS WITH POSSIBLE QUANTUM COMMON CAUSES AND QUANTUM DIRECT CAUSES

A. Possible quantum common causes and quantum direct causes

We review the vector-valued function $\mathbf{P}$ as well as its related properties in [15] first (see Fig. 1). Given a two-qubit system represented by a density operator $\rho$, we measure these two qubits with the same one of three Pauli observables $\sigma_i(i = 1, 2, 3)$ respectively and assume the outcomes are $k$ and $m$ respectively. Then define

$$C_{ii}(\rho) = p(k = m|ii) - p(k \neq m|ii)$$  \hspace{1cm} (1)

and

$$\mathbf{P}(\rho) = \begin{pmatrix} C_{11}(\rho) \\ C_{22}(\rho) \\ C_{33}(\rho) \end{pmatrix}.$$  \hspace{1cm} (2)

When $\rho$ represents an entangled state or a correlated mixture of separable states, it is a common cause. Specially, if $\rho$ is a pure state identified with $|\phi\rangle$ and has a representation in terms of Bell states, i.e., $|\phi\rangle = \sum_{i=1}^{4} w_i |b_i\rangle$, where $\sum_{i=1}^{4} w_i^2 = 1$, $w_i \in \mathbb{R}$ and $|b_i\rangle$ ($i = 1, 2, 3, 4$) is one of the four Bell states, then

$$\mathbf{P}(|\phi\rangle) = \sum_{i=1}^{4} w_i^2 \mathbf{P}(|b_i\rangle).$$  \hspace{1cm} (3)

Except for the quantum common cause, quantum causality is also a possible explanation of the observed quantum correlation. In this case, there is a unitary transformation $U$, i.e., a direct cause, between the measured states of the two qubits (which are actually the same qubit sequentially occurring twice). As in the common cause case, the same measurements are take on the qubit before and after the transformation $U$, to get the statistic $\mathbf{P}$. It was proved in Ref. [15] that the $\mathbf{P}$ value in this case does not depend on the state of the early qubit, but on $U$. Then $\mathbf{P}$ can be regarded as the function of $U$. And we denote it by $\mathbf{P}(U)$. For any given $U$, it was showed that there exist $p_j \geq 0$ satisfying $\sum_{j=0}^{3} p_j = 1$ such that

$$\mathbf{P}(U) = \sum_{j=0}^{3} p_j \mathbf{P}(\sigma_j),$$  \hspace{1cm} (4)

where $\sigma_j (j = 0, 1, 2, 3)$ is one of the four Pauli matrices (including identity matrix $\sigma_0$).

The value of $\mathbf{P}$ can be used to evaluate the existence of quantum causality. However, as stated in the introduction, when the value of $\mathbf{P}$ is in the overlapping area, more designed measurements are needed. To this end, we first analyze the current measurement result, which is represented as Eq. (3) with $w_i$ ($i = 1, 2, 3, 4$) or Eq. (4) with $p_i$ ($i = 0, 1, 2, 3$), to get the general representation forms of possible quantum common causes and possible quantum direct causes. We show them in Lemma 1 and Lemma 2.

Lemma 1. Given $w_j (j = 1, 2, 3, 4) \in \mathbb{R}$ satisfying $\sum_{j=1}^{4} w_j^2 = 1$, if only pure states are considered, there exist and only exist the state

$$|\phi\rangle = \sum_{j=1}^{4} w_j e^{i\theta_j} |b_j\rangle$$  \hspace{1cm} (5)

such that $\mathbf{P}(|\phi\rangle) = \sum_{j=1}^{4} w_j^2 \mathbf{P}(|b_j\rangle)$, where $\theta_j$ called the phase of $w_j$ can be any value in $[0, 2\pi)$. The set of all the above pure states with the same $\mathbf{P}(|\phi\rangle)$ value denotes by $\Phi(w_1, w_2, w_3, w_4)$.
The proof is in the Appendix A.

Obviously, if mixed quantum states as common causes are considered, the mixed quantum states represented as a convex combination of the pure sates in Lemma 1 can also meet the requirement of Lemma 1.

**Lemma 2.** Given \( p_j \geq 0 (j = 0, 1, 2, 3) \) satisfying \( \sum_{j=0}^{3} p_j = 1 \), there exist and only exist \[ U = e^{i \theta} \left( e^{i \tau_1 \cos(\phi_0)} e^{i \tau_2 \sin(\phi_0)} \right) \] such that \( P(U) = \sum_{j=0}^{3} p_j P(j) \), where \( \cos(\phi_0) = \sqrt{c_1} \), \( \sin(\phi_0) = \sqrt{1-c_1} \), \( \gamma_1 = (-1)^{n_1} \arccos(\frac{\tau_1}{\sqrt{2}}) + k_1 \pi \) (if \( c_1 = 0 \), let \( \gamma_1 = 0 \)), \( \gamma_2 = (-1)^{n_2} \arccos(\frac{\tau_2}{\sqrt{2}}) + k_2 \pi \) (if \( d_1 = 0 \), let \( \gamma_2 = 0 \)), \( c_1 = p_0 + p_3 \), \( c_2 = p_0 - p_3 \), \( d_1 = p_1 + p_2 \), \( d_2 = p_2 - p_1 \), \( \frac{\pi}{2} \in [0, \pi] \) is a global phase, and \( n_1, n_2, k_1, k_2 \in \{0, 1\} \). The set of all the above unitary matrices with the same \( P(U) \) value denotes by \( U(p_0, p_1, p_2, p_3) \).

The proof is in the Appendix B.

### B. The changes of \( P \) when the observables are transformed

Based on the analysis results, by applying unitary operators \( V \) on the observables of the two qubits respectively, we are interested in whether there are differences between the changes of the value of \( P \) of the common cause case and that of the causality case, where \( V \in U(2) \) (whose global phase is omitted) is expressed as

\[ V = \left( \begin{array}{cc} e^{i \psi} \cos(\varphi) & e^{i \chi} \sin(\varphi) \\ -e^{-i \chi} \sin(\varphi) & e^{-i \psi} \cos(\varphi) \end{array} \right). \]

These differences may diverge quantum common causes and quantum causality, which is the starting point of our subsequent analysis. We introduce the following definition firstly:

**Definition 1.** Given two qubits represented by a density operator \( \rho \) and a unitary operator \( V \), measuring the observables \( V \sigma V^\dagger \) on the two qubits respectively gives new values of \( P(\rho) \), \( C_{ji}(\rho) \) and the probabilities \( p(k = m|ii) \) as well as \( p(k \neq m|ii) \). Denote them by \( P(\rho) \), \( C_{ji}(\rho) \) and \( p(\rho) \) as well as \( p(\rho) \).

We first discuss the common cause case. Over the set of possible quantum common causes, the general calculation formula of \( P(\rho) \) for any arbitrary unitary operator \( V \) is shown in the following Lemma 3.

**Lemma 3.** Quantum common causes scenario. Given two qubits in the quantum state \( \rho \), for any arbitrary unitary operator \( V \in U(2) \) as stated in Eq. (7),

\[ p(\rho) = \text{Tr} \left( (V \otimes V) \left( \xi^{dd}_{\rho} + \xi^{uu}_{\rho} \right) (V \otimes V) \right) \]

In particular, if \( \rho = |\phi \rangle \langle \phi | \) and \( |\phi \rangle \) is a quantum pure state with \( |\phi \rangle = \sum_{j=1}^{3} w_j e^{i \theta_j} |b_j \rangle \) as stated in Eq. (5), thus

\[ p(\rho) = Tr \left( B'(V \otimes V) \left( \xi^{dd}_{\rho} + \xi^{uu}_{\rho} \right) (V \otimes V) \right) \]

where \( \xi^{uu} \) and \( \xi^{dd} \) are spectral measures associated to the observable \( \sigma_i \otimes \sigma_i (i = 1, 2, 3) \), reflecting whether both qubits are pointing the same direction, \( B' = (|b_1 \rangle \langle b_1|, |b_2 \rangle \langle b_2|, |b_3 \rangle \langle b_3|, |b_4 \rangle \langle b_4|) \) and \( w = (w_1 e^{-i \theta_1}, w_2 e^{-i \theta_2}, w_3 e^{-i \theta_3}, w_4 e^{-i \theta_4})' \).

The proof is in the Appendix C.

As a special case of Lemma 3, we give the following corollary for the computation of \( C_{33|V} \) on particular pure states with \( w_4 = 0 \) since Our many following works are in large part associated with the analysis of the changes of the value of \( C_{33|V} \).

**Corollary 3.1.** Specially, given \( |\phi \rangle = \sum_{j=1}^{3} w_j e^{i \theta_j} |b_j \rangle \) with \( w_4 = 0 \), after having applied unitary operation \( V \) on the observables of the two qubits respectively, We have

\[ C_{33|V} (|\phi \rangle) = C_{33}(V \otimes V)' (|\phi \rangle) \]

In particular, if \( \rho = |\phi \rangle \langle \phi | \) and \( |\phi \rangle \) is a quantum pure state with \( |\phi \rangle = \sum_{j=1}^{3} w_j e^{i \theta_j} |b_j \rangle \) as stated in Eq. (5), thus

\[ p(\rho) = Tr \left( B'(V \otimes V) \left( \xi^{dd}_{\rho} + \xi^{uu}_{\rho} \right) (V \otimes V) \right) \]

where \( \xi^{uu} \) and \( \xi^{dd} \) are spectral measures associated to the observable \( \sigma_i \otimes \sigma_i (i = 1, 2, 3) \), reflecting whether both qubits are pointing the same direction, \( B' = (|b_1 \rangle \langle b_1|, |b_2 \rangle \langle b_2|, |b_3 \rangle \langle b_3|, |b_4 \rangle \langle b_4|) \) and \( w = (w_1 e^{-i \theta_1}, w_2 e^{-i \theta_2}, w_3 e^{-i \theta_3}, w_4 e^{-i \theta_4})' \).

The proof is in the Appendix C.

As a special case of Lemma 3, we give the following corollary for the computation of \( C_{33|V} \) on particular pure states with \( w_4 = 0 \) since Our many following works are in large part associated with the analysis of the changes of the value of \( C_{33|V} \).

**Corollary 3.2.** Given \( w_j \in \mathbb{R} (j = 1, 2, 3, 4) \) as stated in Lemma 1, for \( \forall |\phi \rangle \in \Phi(|w_1, w_2, w_3, w_4|) \) and \( \forall V \in U(2) \) as stated in Eq. (7), \( P(\rho) \) takes values in a fixed plane. The plane is determined only by \( \{w_j | j = 1, 2, 3, 4\} \) and is independent of the choice of \( V \) and the phase of \( w_j (j = 1, 2, 3, 4) \).

The proof is in the Appendix D.
Lemma 4. Quantum causality scenario. Given $U \in \mathcal{U}(p_0, p_1, p_2, p_3)$ as stated in Eq. (6) and $V \in \mathcal{U}(2)$ as stated in Eq. (7), applying $V$ in temporal order on the observables of the two qubits respectively, then $P_V(U) = P(V'UV)$. Further, $C_{11, V}(U) = 2(a_1^2 + b_2^2) - 1$, $C_{22, V}(U) = 2(a_1^2 + b_2^2) - 1$ and $C_{33, V}(U) = 2(a_1^2 + b_2^2) - 1$, wherein $a_1 = \cos(\phi_0) \cos(\gamma_1), a_2 = \cos(\phi_0) \cos(2\phi) \sin(\gamma_1) - \sin(\phi_0) \sin(2\phi) \sin(\gamma_2 - \psi - \chi), b_1 = \sin(\phi_0) \cos^2(\phi) \cos(\gamma_2 - 2\psi) + \sin(\phi_0) \sin^2(\phi) \cos(\gamma_2 - 2\psi) - \cos(\phi_0) \sin(2\phi) \sin(\gamma_2 - \psi - \chi)), b_2 = - \sin(\phi_0) \sin^2(\phi) \sin(\gamma_1), b_3 = \sin(\phi_0) \cos^2(\phi) \sin(\gamma_2 - 2\psi) + \cos(\phi_0) \sin(2\phi) \cos(\gamma_1 - \psi) \sin(\gamma_1)$.

The proof is in the Appendix E.

Corollary 4.1. Given $p_j \geq 0(j = 0, 1, 2, 3)$ as stated in Lemma 2 and $V \in \mathcal{U}(2)$, the image set of $P_V(U)(U \in \mathcal{U}(p_0, p_1, p_2, p_3))$ contains at most four different elements.

The proof is in the Appendix F.

Next, just like the quantum common cause case, we find for any possible direct cause behind the initial value of $P$ and for any unitary operator $V$, $P_V$ also lie in a fixed plane (see Fig. 2).

Corollary 4.2. Given $p_j \geq 0(j = 0, 1, 2, 3)$ as stated in Lemma 2, for all $U \in \mathcal{U}(p_0, p_1, p_2, p_3)$ and all $V \in \mathcal{U}(2)$ as stated in Eq. (7), $P_V(U)$ takes values in a fixed plane. The plane is determined only by $\{p_j \mid j = 0, 1, 2, 3\}$ and is independent of the choice of $V$.

The proof is in the Appendix G.

Finally, we show that the plane mentioned in Corollary 3.2 is identical to the plane stated in Corollary 4.2 when the value of $P$ discussed in the two corollaries are the same. This property motivates us to discuss the discrimination problem plane by plane (see the next subsection).

We summarize the corresponding results as Lemma 5 and Lemma 6, wherein the quantum-common-cause part of Lemma 5 only discusses the pure quantum states and Lemma 6 discusses the general case, i.e., general quantum common causes including mixed quantum states.

Lemma 5. Analyzing the initial given value of $P$ to get $\Phi(w_1, w_2, w_3, w_4)$ and $U(p_0, p_1, p_2, p_3)$, then for all $V \in \mathcal{U}(2)$, $P_V(\Phi)$ and $P_V(U)$ are always lying in the same plane, where $P(\Phi)$ and $P(U)$ respectively the image sets of $P$ over the set $\Phi$ and $U$. The plane’s norm vector is $(1, 1, 1)^T$ and its const term ranges from $-1$ to 1.

The proof is in the Appendix H.

Definition 2. We denote the const term $4p_0 - 1$ or $1 - 4w_4^2$ by $b$. And since these planes differ from each other only by the const term, we use $l(b)$ to represent the plane with the const term $b$.

Lemma 6. Given an initial measurement result of $P$ of two qubits in the plane $l(b)$, with any arbitrary unitary operator $V$, for any possible common cause $\rho$ and for any possible direct cause $U$, $P_V(\rho)$ and $P_V(U)$ are still in the plane $l(b)$ (see Fig. 2).

FIG. 2. The geometric interpretation of the range of the value of $P_V$. Given an initial value of $P$(represented by the black symbol ’*’) in the plane $l(b)$, analyze the current value of $P$ to get a possible common cause $\rho$ and a possible direct cause $U$. Then with some arbitrary unitary operations $V$, the values of $P_V(\rho)$ (represented by the symbol ’.’) lie in the intersection area of TCC and the plane $l(b)$, i.e., the triangle with vertices A, B, C; the values of $P_V(U)$ (represented by the symbol ‘+’ ) lie in the intersection area of TDC and the plane $l(b)$, i.e., the triangle with vertices D, E and F.

The proof is in the Appendix I.

III. DESIGN OF UNITARY OPERATORS

In this section, we show how to design unitary operators to get appropriate $P_V$ functions for the discrimination task. It can be seen from Lemma 5 and 6 that no matter what unitary matrix is chosen, $P_V$ is always in the $l(b)$ plane that $P$ is initially in. This prompt us to take the area that is in the plane and in which the respective value of $P_V$ of quantum common causes and quantum direct causes do not overlap as the target of $P_V$.

Compared to the difficulty to handle the infinite cases of possible quantum common causes, it is relatively easy to deal with the possible 16 cases of quantum causality (see Theorem 1 below). Furthermore, by Lemma 4, $C_{33, V}$ is formally simpler than $C_{11, V}$ and $C_{22, V}$. And we notice that given $P$ in the plane $l(b)(b \neq 1)$, among the points that belong to the image set of $P_V(U)(U \in \mathcal{U}), P_V$ with $C_{33, V}$ being 1 is one of the possible points that are farthest from the image set of $P_V(\langle \phi \rangle |\langle \phi \rangle \in \Phi)$ (see Fig. 2). Based on the above considerations, the design of unitary operators aims to transfer the third entry of $P_V$, i.e., $C_{33, V}$ to 1 when there is a causality between the two qubits. To implement this idea, two questions need to be answered. The first question is that given an initial value of $P$, whether there are appropriate operators $V$ such that for all possible cases of quantum causality, $C_{33, V}$ are equal to 1. The second question is whether we can conclude there exists a quantum causality when $C_{33, V}$ is equal to 1.
As presented in Corollary 4.1, given \( p_j \geq 0 (j = 0, 1, 2, 3) \), \( U(p_0, p_1, p_2, p_3) \) can be divided into four subsets according to the values of \( P \) on them. The four subsets denote by \( U_k(p_0, p_1, p_2, p_3)(k = 1, 2, 3, 4) \). For the first question, we first prove that with carefully designed unitary operators acting on the observables, the third entry of \( P \) \((k = 1, 2, 3, 4)\) can be equal to 1 (see Fig. 3). For the second question, we prove for any possible quantum common cause \( \rho \), with any unitary operator \( V \), the entries of \( P \) \((k = 1, 2, 3, 4)\) can not be equal to 1, unless \( P \) is initially in the plane \( l(1) \)(see Fig. 3). The results are shown in Theorem 1 and Theorem 2.

**Theorem 1.** Given \( p_j (j = 0, 1, 2, 3) \) and \( k \in \{1, 2, 3, 4\} \), for \( \forall U \in U_k(p_0, p_1, p_2, p_3) \), there exist unitary operators \( V \) as stated in Eq. (7) with

\[
\psi + \chi = \gamma_2 - \frac{k_1 \pi}{2}, \varphi = \frac{k_2 \pi - \omega}{2},
\]

such that \( P(V)(U) = (2p_0 - 1, 2p_0 - 1, 1)' \), where \( \sin(\omega) = \sin(\gamma_0) \sin(\gamma_2 - \varphi - \chi), \cos(\omega) = \cos(\gamma_0) \sin(\gamma_2) \) and \( r = \sqrt{\cos^2(\gamma_0) \sin^2(\gamma_1) + \sin^2(\gamma_0) \sin^2(\gamma_2 - \varphi - \chi)} \); \( \gamma_0, \gamma_2 \) and \( \gamma_2 \) are the parameters of \( U \) (see Lemma 2); \( k_1 = 1, 2 \) and \( k_2 = 1, 2 \).

The proof is in the Appendix J.

It is easy to check that with different values of \( k_1 \) and \( k_2 \) of \( V \), the obtained values of \( C_{33,V}(\{\phi\}) \) are the same. Due to this reason, we do not differentiate between the values of \( k_1 \) as well as \( k_2 \) in the following. Moreover, it is worth to note that for any given \( U_k \), the number of satisfied \( V \) is infinite since there are only two necessary restrictions imposed on the three free parameters of \( V \) to promise \( C_{33,V}(U) = 1 \). And by Corollary 3.1, the value of \( C_{33,V}(\{\phi\}) \) does also not depend on the respective \( \psi \) or \( \chi \) but on the sum of them (which holds also for quantum mixed states since quantum mixed states can be seen as a convex combination of pure quantum states). So it seems that we need not to care the individual values of \( \psi \) or \( \chi \). However, we show specifying a special value of \( \chi \) or \( \psi \) for \( V \) can facilitate the discrimination task when \( P \) is initially in the plane \( l(1) \) (see the discussion after Theorem 3). The set of all the satisfied \( V \) for \( U_k \) is denoted by \( V^k \). And the collection of \( V^k(k = 1, 2, 3, 4) \) is denoted by \( V \), i.e., \( V = \{V^k|k = 1, 2, 3, 4\} \).

**Theorem 2.** Given two qubits in the state \( \rho \), no unitary matrix \( V \in U(2) \) can make any entry of \( P(V)(\rho) \) be 1, unless \( P(V)(\rho) \) is in the plane \( l(1) \).

The proof is in the Appendix K.

As a special case of Theorem 1, when \( P \) is initially in the plane \( l(1) \), \( P(V)(U) \) is \( (0, 0, 1)' \) by the obtained \( V \). However, in this case, \( P(V)(\rho) \) can also be \( (0, 0, 1)' \), which may cause the discrimination task to fail. We discuss this special case in Theorem 3 and show the conditions under which the obtained \( V \) can still work to promise \( P(V)(\rho) \) not to be \( (0, 0, 1)' \) (see Fig. 4).

![FIG. 3. The cases where \( P \) is initially in \( l(b)(b \neq 1) \). Given the statistic \( P \) (represented by the black symbol ‘+’) of two qubits in the plane \( l(b)(b \neq 1) \), if there is a direct cause \( U \in U_k(k = 1, 2, 3, 4) \) between the two qubits, then for \( \forall V \in V^k \), \( P(V) \) is transferred to the point \( F \) with third entry being 1. However, if the two qubits have a common cause acting on them, then for \( \forall V(k = 1, 2, 3, 4) \) and \( V' \in V^k \), \( P(V') \) (represented by the red symbol ‘−’) is not equal to the point \( F \).](image)

**Theorem 3.** Given \( P \neq (0, 0, 1) \) in the plane \( l(1) \), analyzing current \( P \) can obtain \( U_k(p_0, p_1, p_2, p_3)(k = 1, 2, 3, 4) \) and the corresponding \( V \) as stated above. For any quantum state \( \rho \) satisfying \( P(\rho) = P \) and \( \forall V \in V^k(k = 1, 2, 3, 4) \), \( P(V)(\rho) \neq (0, 0, 1)' \) holds unless that \( f_2 = \sin(2\chi - 2\psi) = 0 \) or \( f_2 = f_3 = 0 \), where \( \psi \) and \( \chi \) are parameters of \( V \) as stated in Eq. (7), \( f_3(i = 1, 2, 3) \in \mathbb{R} \) are parameters of \( \rho \) and

\[
\rho_v = (V \otimes V)' \rho (V \otimes V) = \begin{pmatrix}
0 & 0 & f_2 - i f_3 \\
0 & 0 & 0 \\
f_2 + i f_3 & 0 & 1 - f_1
\end{pmatrix}.
\]
results of quantum direct cause when their $P$ are originally the same. Recall that the value of $P_V$ is restricted to the same plane $l(b)$ when only applying a single $V$ on the observables of the two qubits respectively; that only in the plane $l(1)$, $P_V(\rho)$ may be $(0,0,1)'$. Then a feasible solution to this case may be applying different unitary operators on the observables of one qubit and another qubit respectively to transfer current $P$ to another plane $l(b)(b \neq 1)$. We choose the plane $l(-1)$ as the destination plane because in the plane, the corresponding destination point $(-1,-1,1)'$ is far from the image set of $P_V(\rho)$, which may help to reduce the uncertainty caused by the quantum mechanism in the discrimination process. In addition, we only consider how to transfer $P = (0,0,1)'$ to the plane $l(-1)$ since $P$ can always be transferred to $(0,0,1)'$ first in this case and the analysis process is relatively simpler when compared with the cases that $P$ is not $(0,0,1)'$. We have the following theorem.

**Theorem 4.** Let $V_\perp$ be an identity matrix and

$$V_\perp = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{13}$$

Given two qubits either in the quantum state $\rho$ or existing a direct cause $U$ between them, where $\rho$ is stated as in Eq. (12) with $f_2 = f_3 = 0$ and $U$ satisfies $P(U) = (0,0,1)'$, after having applied $V_\perp$ and $V_\parallel$ on the observables of the two qubits in temporal order, then measuring these new observables gives new values of $P$, which are in the plane $l(-1)$.

The proof is in the Appendix M.

Once $P$ is transferred to the plane $l(-1)$, we can conveniently use Theorem 1 and Theorem 2 to distinguish quantum direct causes from quantum common causes.

**IV. DISCRIMINATION METHOD**

Based on the above theoretical observations, we develop a method for the discrimination task by using experimental observations only. Supposing we have prepared many copies of a system to be tested, we measure the same Pauli observables on the two qubits before unitary transformation to get the estimated values of $P$ and measure the transformed Pauli observables on the two qubits to get the estimated values of $P_V$ if it is necessary. With the estimated values of $P$ and $P_V$, we identify whether there are causalities between the two qubits or not. It contains the following steps (see Fig. 5):

1. Measure the same Pauli observable $\sigma_i(i = 1,2,3)$ on the two qubits to get the estimated value of $P$.
2. If the estimated value of $P$ is outside of the overlapping area, it is the end; if the estimated value of $P$ is $(0,0,1)'$, then apply a unitary operation $V_0$ as stated in the discussion after Theorem 3 on the observables of the two qubits first to get new observables and new $P$ whose third entry is no longer 1; else, go to the next step.
3. Using Eq. (6) to obtain the set of possible cases of quantum causality, i.e., $U(p_0, p_1, p_2, p_3)$.
4. Following from Corollary 3.1, divide $U$ into four subsets $U_k(k = 1,2,3,4)$. For every $U_k(k = 1,2,3,4)$, by Eq. (11) in Theorem 1, design one group of unitary matrices $V_k$.
5. For $\forall k \in \{1,2,3,4\}$, pick one $V_k \in V_k$ with $0 < \chi - \psi < \frac{\pi}{2}$ at random; apply it on the current observables to get the estimated value of $P_V$ denoted by $P_k^e$.
6. If there exists a $k \in \{1,2,3,4\}$ such that $P_k^e = (0,0,1)'$, then after having applied $V_k$ on the current two observables, apply $V_\perp$ and $V_\parallel$ as stated in Theorem 4 on the current observables to get new observables and new value of $P$; go to the next step. Otherwise, if there exists a $k \in \{1,2,3,4\}$ such that the third entry of $P_k^e$ is 1 and its first two entries are equal, then there is a direct causal connection between the two qubits; else there is a common cause acting on them.
7. For the current observables and the current value of $P$, perform steps (3) through (5) to get the new value of $P_k^e$. If there exists a $k \in \{1,2,3,4\}$ such that the third entry of $P_k^e$ is 1, then there is a direct causal connection between the two qubits; else there is a common cause acting on them.

Simulation experiments were conducted on the systems with the parameters of the quantum states (common causes) and the unitary matrices (direct causes) randomly sampled from their legal intervals. For each measurement, we simulated it by sampling 200 examples from $P$ or $P_V$ (which actually includes 3 distributions) thereby getting the estimated value of $P$ or $P_V$. In total, we created 1e4 quantum states and 1e4 unitary matrices respectively. The tolerance of the algorithm was set as 1-c1, which means that if $|a - b| < 1 - c1$, we argue $a = b$. Each experiment was repeated five times. The average number of failed cases is 251(±10), accounting for 1.26%(±0.05%). And when the number of sampling
increased to more than 800, no failure cases were observed.

V. CONCLUSIONS AND FUTURE WORKS

The possibility of intervening is requisite for causal reasoning of classical causal models. However, the interventionist schemes cannot be directly applied to the quantum case. The dilemma is presented as a choice between relinquishing one of two assumptions: the Causal Markov Condition or faithfulness (no-fine-tuning) [16]. Instead of trying to modify one of the existing assumptions, another probably better approach to avoid such dilemma is reformulating causal models in a way that makes direct use of the quantum formalism and providing a quantum interventionist framework for Bayesian inference as well as causal inference [17].

In this paper, distinct from the quantum interventionist framework, we adopt the frequentist manner and prove that quantum observation schemes can universally identify causalities from correlations. We first analyze the manner in which the statistic \( P \) moves when the observables are transformed by unitary operations. Using this obtained property, we show how to design unitary matrices to make quantum common causes and quantum causality be distinguishable. A discrimination method is developed and is testified by simulation. Nonetheless, the mixture case of quantum common causes and quantum direct causes may also account for the observed correlation, which was not discussed in this paper. We leave its analysis and the development of corresponding discrimination method in the future work.

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Appendix A: PROOF OF LEMMA 1

Proof. On the one hand, a straightforward calculation can show

\[
P(\phi) = \sum_{i=1}^{4} w_i^2 P(b_i)
\]

holds for \( \phi = \sum_{j=1}^{4} w_j e^{i\theta_j} |b_j\rangle \). Then the existence is proved. On the other hand, \( \{ P(b_i) \mid i = 1, 2, 3, 4 \} \) form a complete basis; if there exists another group of coefficients \( \{ v_j \mid j = 1, 2, 3, 4, v_j \in \mathbb{C} \} \) such that \( |\phi\rangle = \sum_{j=1}^{4} v_j |b_j\rangle \) satisfies Eq. (A1), thus \( |v_j|^2 = w_j^2 \). Then the uniqueness is proved.

□
Appendix B: PROOF OF LEMMA 2

Proof. Let

\[ U_x = \begin{pmatrix} a_1 + ia_2 & b_1 + ib_2 \\ -e^{i\alpha}(b_1 - ib_2) & e^{i\alpha}(a_1 - ia_2) \end{pmatrix} \]  

be an arbitrary unitary matrix in U(2), where \( a_1^2 + a_2^2 + b_1^2 + b_2^2 = 1 \). As proved in Ref. [15],

\[ \mathbf{P}(U_x) = \begin{pmatrix} 2(c - d) - 1 \\ 2(c + d) + 1 \\ 2(a_1^2 + a_2^2) - 1 \end{pmatrix} \]  

(B2)

where \( c = \frac{1}{2} + a_1a_2 \sin \alpha + \frac{\cos \alpha}{2} (a_1^2 - a_2^2) \), \( d = b_1b_2 \sin \alpha + \frac{\cos \alpha}{2} (b_1^2 - b_2^2) \). Plug \( U \) defined in Eq. (6) into above Eq. (B2), it is easy to find

\[ \mathbf{P}(U) = \sum_{j=0}^{3} p_j \mathbf{P}(\sigma_j) \]  

(B3)

holds, i.e., the existence of \( U \) is proved, where \( \mathbf{P}(\sigma_0) = (1, 1, 1) \), \( \mathbf{P}(\sigma_1) = (1, -1, -1) \), \( \mathbf{P}(\sigma_2) = (-1, 1, -1) \), \( \mathbf{P}(\sigma_3) = (-1, -1, 1) \). Next to prove the uniqueness of \( U \). Supposing an unknown \( U_x \) satisfies above Eq. (B3), then

\[ \begin{cases} \sin \alpha (a_1^2 - a_2^2) + p_0 - p_3 \\ a_1^2 + a_2^2 - p_0 + p_3 \\ b_1b_2 \sin \alpha + (b_1^2 - b_2^2) = p_2 - p_1. \end{cases} \]  

(B4)

If \( p_0 + p_3 = 0 \) or \( p_1 + p_2 = 0 \), we have \( a_1 = a_2 = 0 \) or \( b_1 = b_2 = 0 \). Otherwise, let \( c_1 = p_0 + p_3 \), \( c_2 = p_0 - p_3 \), \( d_1 = p_1 + p_2 \), \( d_2 = p_2 - p_1 \), \( \cos \xi_1 = \frac{\sqrt{c_1}}{\sqrt{c_2}} \), \( \cos \xi_2 = \frac{\sqrt{c_1}}{\sqrt{d_2}} \), \( \sin \xi_1 = \frac{\sqrt{c_2}}{\sqrt{c_1}} \), \( \sin \xi_2 = \frac{\sqrt{d_2}}{\sqrt{c_1}} \); plug these equations into above Eq. (B4) and assume \( \alpha = \theta \) is known, thus \( \xi_1 = \gamma_1 + \frac{\theta}{2}, \xi_2 = \gamma_2 + \frac{\theta}{2}, \) where \( \gamma_1 = (1)^{n_1} \arccos \left( \frac{c_2}{d_2} \right) + k_1 \pi, \gamma_2 = (1)^{n_2} \arccos \left( \frac{c_1}{d_1} \right) + k_2 \pi \) and \( n_1, n_2, k_1, k_2 \in \{0, 1\} \).

Appendix C: PROOF OF LEMMA 3

Proof. After having applied unitary evolution \( V \otimes V \) on the observable \( \sigma_i \otimes \sigma_i \), the probability of finding both qubits in the same direction is

\[ p_i(k = m|ii) = \text{Tr} \left( (V \otimes V) \left( \xi_i^{dd} + \xi_i^{uu} \right) (V \otimes V) \right) \rho \]

\[ = \text{Tr} \left( (V \otimes V) (\xi_i^{dd} + \xi_i^{uu}) (V \otimes V) \right) \langle \phi | \langle \phi \right) \]

\[ = \text{Tr} \left( B' (V \otimes V) (\xi_i^{dd} + \xi_i^{uu}) (V \otimes V) (\xi_i^{dd} + \xi_i^{uu}) B' \right). \]  

(C1)

Appendix D: PROOF OF COROLLARY 3.2

Proof. We only need to prove that the sum of the three entries of \( \mathbf{P}_V (|\phi \rangle) \) is a fixed value independent of \( V \) as well as the phase of \( w_j (j = 1, 2, 3, 4) \).

\[ C_{11,V}(|\phi \rangle) + C_{22,V}(|\phi \rangle) + C_{33,V}(|\phi \rangle) \]

\[ 2 \left( \sum_{i=1}^{3} p_i (k = m|ii) \right) = 0. \]

\[ 2 \text{Tr} \left( (B^T (V \otimes V) \sum_{i=1}^{3} (\xi_i^{dd} + \xi_i^{uu}) (V \otimes V) Bw) \right) = 3. \]  

(D1)

After careful calculation, it is easy to find

\[ (B^T (V \otimes V) \sum_{i=1}^{3} (\xi_i^{dd} + \xi_i^{uu}) (V \otimes V) Bw) = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \]  

(D2)

Plug Eq. (D2) into Eq. (D1), we have

\[ C_{11,V}(|\phi \rangle) + C_{22,V}(|\phi \rangle) + C_{33,V}(|\phi \rangle) = 4 \sum_{i=1}^{3} w_i^2 - 3 = 1 - 4w_i^2. \]  

(D3)

Appendix E: PROOF OF LEMMA 4

Proof. It has been shown in Ref. [15] that \( \mathbf{P}_V(U) = \mathbf{P}(V^\dagger UV) \). Further, let \( V^\dagger UV \) be \( \begin{pmatrix} a_1 + ia_2 & b_1 + ib_2 \\ b_1 - ib_2 & a_1 - ia_2 \end{pmatrix} \), then \( a_1, a_2, b_1 \) and \( b_2 \) would take values as given in the Lemma 4. Finally, by Eq. (B2), \( C_{ii,V}(V^\dagger UV) \) for \( i = 1, 2, 3 \), i.e., \( C_{ii,V}(V^\dagger UV) \) can be expressed as the function of \( a_1, a_2, b_1 \) and \( b_2 \) as stated in Lemma 4.

Appendix F: PROOF OF COROLLARY 4.1

Proof. From Lemma 2, we see that \( U(p_0, p_1, p_2, p_3) \) contains 16 unitary matrices (whose global phases are omitted), each of which is determined by \( (n_1, n_2, k_1, k_2) \). Further, it is easy to see that the unitary matrix determined by \( (1 - n_1, n_2, 1 - k_1, k_2) \) is the same as the unitary matrix determined by \( (n_1, n_2, k_1, k_2) \); and the unitary matrix determined by \( (n_1, n_2, 1 - k_1, 1 - k_2) \) differs from that determined by \( (n_1, n_2, k_1, k_2) \) only by the sign. Moreover, following from Lemma 4, \( \mathbf{P}_V(-U) = \mathbf{P}_V(U) \) holds. Thus, \( U(p_0, p_1, p_2, p_3) \) can be divided into four subsets. Over each subset, the values of \( \mathbf{P}_V(U) \) are the same.

Appendix G: PROOF OF COROLLARY 4.2

Proof. We only need to prove that the sum of the three entries of \( \mathbf{P}_V(U) \) is a fixed value independent of \( V \). Following from Lemma 4 and by the fact that \( a_1^2 + a_2^2 + b_1^2 + b_2^2 = 1 \), we get \( C_{11,V}(U) + C_{22,V}(U) + C_{33,V}(U) = 4a_1^2 - 1 \). Finally, by Lemma 2, we have \( a_1^2 = \cos(\phi_0) \cos(\gamma_1) = p_0 \) is dependent of the choice of \( V \).

\[ \square \]
Appendix H: PROOF OF LEMMA 5

Proof. Corollary 3.2 and Corollary 4.2 have showed the norm vectors of the discussed planes in the two cases are all $\langle 1, 1, 1 \rangle$, thus what we need to prove is the constant terms of the two planes are actually equal. In fact, because $\Phi(w_1, w_2, w_3, w_4)$ and $U(p_0, p_1, p_2, p_3)$ are the analysis results of the same value of $\mathbf{P}$, then for $\forall \langle \phi \rangle \in \Phi(w_1, w_2, w_3, w_4)$ and for $\forall U \in U(p_0, p_1, p_2, p_3)$, we have $\mathbf{P}(\langle \phi \rangle) = \mathbf{P}(U)$ thereby getting $e\mathbf{P}(\langle \phi \rangle) = e\mathbf{P}(U)$, where $e = (1, 1, 1)$. By Corollary 3.2 and Corollary 4.2, we obtain $4p_0 - 1 = 4 - 4w^2$. That’s to say the two planes have the same constant term. Further, $p_0$ and $w^2$ are all non-negative, so the range of the constant term must be $[-1, 1]$.

Appendix I: PROOF OF LEMMA 6

Proof. According to the Lemma 5, we only need to prove it holds for mixed quantum states. In fact, When $\rho$ is a mixed state, $\mathbf{P}(\rho)$ and $\mathbf{P}_V(\rho)$ can be respectively regarded as a convex combination of $\mathbf{P}(\rho_i)(i = 1, 2, ..., N)$ and a convex combination of $\mathbf{P}_V(\rho_i)(i = 1, 2, ..., N)$ with the same combinatorial coefficients, where $\rho_i(i = 1, 2, ..., N)$ is a pure state and $N$ is the number of pure states. Because by Lemma 5, $\mathbf{P}_V(\rho_i)$ and $\mathbf{P}(\rho_i)$ are all in the same plane $l(b_i)$ (supposing $\mathbf{P}(\rho_i)$ is initially in the plane $l(b_i)$), then the respective combinations of them with the same combinatorial coefficients should be in the same plane $l(b)$.

Appendix J: PROOF OF THEOREM 1

Proof. Recall that $\mathbf{P}_V(U) = \mathbf{P}(V'UV)$ should lie in the regular tetrahedron (denoted by TCC) with vertices $\mathbf{P}(\sigma_0) = (1, 1, 1)', \mathbf{P}(\sigma_1) = (1, -1, -1)', \mathbf{P}(\sigma_2) = (-1, 1, -1)'$ and $\mathbf{P}(\sigma_3) = (-1, -1, 1)'$. Also, According to Corollary 4.2, $\mathbf{P}_V(U)$ should be in the plane $l(4p_0 - 1)$. The intersection of them is a triangle with vertices $(1, 2p_0 - 1, 2p_0 - 1)', (2p_0 - 1, 1, 2p_0 - 1)'$ and $(2p_0 - 1, 1, 2p_0 - 1)'$. Also, the other two entries must be $2p_0 - 1$.

Next, we prove there exists $V$ as stated in Eq. (7) such that $C_{33V}(U) = 1$, where $U \in U_k$ is given as in Eq. (6). It has been presented in Lemma 4 that $C_{33V}(U) = 2(a_1^2 + a_2^2) - 1$, where $a_1 = \cos(\phi_0) \cos(\gamma_1)$ and $a_2 = \cos(\phi_0) \cos(\gamma_1)\sin(\gamma_1) - \sin(\phi_0) \sin(\gamma_2 + \phi - \phi_1) = r \cos(2\phi + \omega)$.

where

$$r = \sqrt{\cos^2(\phi_0) \sin^2(\gamma_1) + \sin^2(\phi_0) \sin^2(\gamma_2 - \psi - \phi)}, \quad (J2a)$$

$$\sin(\omega) = \frac{\sin(\phi_0) \sin(\gamma_2 - \psi - \phi)}{r}, \quad (J2b)$$

$$\cos(\omega) = \frac{\cos(\phi_0) \sin(\gamma_1)}{r}. \quad (J2c)$$

Because $|\cos(2\phi + \omega)| \leq 1$, we must promise $r^2 \geq 1 - a_1^2$ to get $a_1^2 + a_2^2 = 1$. Simplifying $r^2 \geq 1 - a_1^2$, we get its equivalent form

$$\sin^2(\gamma_2 - \psi - \phi) \geq 1. \quad (J3)$$

That’s to say $r^2 \geq 1 - a_1^2$ is possible only when $\psi + \chi = \gamma_2 - \frac{k_1 \pi}{2}$. \quad (J4)

where $k_1 = 1, 3$. At this moment, $1 - a_1^2$ is in fact the maximum value of $r^2$. Consequently, it demands $|\cos(2\phi + \omega)| = 1$, i.e., $\phi = \frac{k_2 \pi - \omega}{2}$. \quad (J5)

where $k_2 = 0, 1$. Taken together, the legal $V$ should meet the Eq. (J4) and Eq. (J5) simultaneously.

Appendix K: PROOF OF THEOREM 2

Proof. If $\rho$ is a pure quantum state, denote it by $|\phi\rangle$ and suppose $|\phi\rangle \in \Phi(w_1, w_2, w_3, w_4)$, where $w_j \in \mathbb{R}(j = 1, 2, 3, 4)$ and $\sum_{j=1}^{4}w_j^2 = 1$. Recall that $\mathbf{P}_V(|\phi\rangle) = \mathbf{P}(\sqrt{V} \otimes V'\sqrt{\phi})$ should lie in the regular tetrahedron (denoted by TCC) with vertices $\mathbf{P}(|b_1\rangle) = (1, -1, 1)', \mathbf{P}(|b_2\rangle) = (-1, 1, 1)', \mathbf{P}(|b_3\rangle) = (1, 1, -1)'$ and $\mathbf{P}(|b_4\rangle) = (-1, -1, -1)'$. Meanwhile, as presented in Corollary 3.2, $\mathbf{P}_V(|\phi\rangle)$ should also be in the plane $l(1 - 4w_4^2)$. The intersection of TCC and $l(1 - 4w_4^2)$ is a triangle with vertices $(-1, 1, 1, 1, 1, 1, 1, 1)'$ and $(-1, 1, 1, 1, 1, 1, 1, 1)'$. Obviously, any linear combination of the three vertices can not be a vector with any entry being 1, unless $w_4 = 0$, i.e., unless $\mathbf{P}(|\phi\rangle)$ is in the plane $l(1)$.

If $\rho$ is a mixed quantum state, it is easy to check $\mathbf{P}_V(\rho)$ is a convex combination of $\mathbf{P}_V(\rho_i)(i = 1, 2, ..., N)$, where $\rho_i$ is a pure quantum state and $N$ is the number of pure quantum states. Since except the case that $\mathbf{P}(\rho_i)$ is in the plane $l(1)$, any entry of $\mathbf{P}_V(\rho_i)$ is not 1, we have any entry of $\mathbf{P}_V(\rho)$ that is the convex combination of $\mathbf{P}_V(\rho_i)$ should not be 1, unless $\mathbf{P}(\rho)$ is in the plane $l(1)$.

Appendix L: PROOF OF THEOREM 3

Proof. We first prove that if $\mathbf{P}(\rho_\nu) = (0, 0, 1)'$, $\rho_\nu = (V \otimes V) \rho (V \otimes V)$ can be expressed as

$$
\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
f_2 + if_3 & 0 & 0 & 1 - f_1
\end{pmatrix}.
$$

\quad (L1)
Here, $\rho_V$ may be a mixed quantum state. And suppose it is a convex combination of pure quantum states $\rho_j (j = 1, 2, ..., N)$, where $\rho_j = |\phi_j\rangle\langle\phi_j|$, $|\phi_j\rangle = \sum_{k=1}^4 w_{jkl} e^{i\theta_{jkl}} |b_k\rangle$, $\theta_{j1} = 0$ (which is treated as a global phase) and $N$ is the number of pure quantum states. Because $P(\rho_V)$ is at the boundary of the legal convex region, $P(\rho_j)$ should also be at the boundary thereby with $w_{j3} = w_{j4} = 0$ for $\forall j \in 1, 2, ..., N$. Then a straightforward computation leads to

$$\rho_j = |\phi_j\rangle\langle\phi_j| = \begin{pmatrix}
 f_{j1} & 0 & 0 & f_{j2} - i f_{j3} \\
 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 \\
 f_{j2} + i f_{j3} & 0 & 0 & 1 - f_{j1}
\end{pmatrix}, \quad (L2)$$

where

$$f_{j1} = (w_{j1}^2 + w_{j2}^2 + 2w_{j1}w_{j2} \cos(\theta_{j2})) / 2 \quad (L3a)$$
$$f_{j2} = (w_{j1}^2 - w_{j2}^2) / 2 \quad (L3b)$$
$$f_{j3} = w_{j1}w_{j2} \sin(\theta_{j2}) \quad (L3c)$$

Thus $\rho_V$, as a convex combination of $\rho_j (j = 1, 2, ..., N)$, can be expressed as in above Eq. (L1).

Next, we prove that $f_2 = f_3 = 0$ or $f_2 = \sin(2\chi - 2\psi) = 0$ is a necessary condition for the equation $P_V(\rho) = (0, 0, 1)'$ to hold. First, we prove $f_2 = 0$ if $P(\rho_V) = (0, 0, 1)'$. In fact, by Lemma 3, we have $P(\rho_V) = (-2f_2, -2f_2, 1)'$ thereby getting $f_2 = 0$ soon. Supposing $P(U) = (0, 0, 1)'$, by Lemma 2, $\gamma_1, \gamma_2$ and $\varphi_0$ of $U$ should be $(-1)^{n_2k_1} \pi + k_1 \pi, 0$ and 0 respectively, where $n_2, k_1 \in \{0, 1\}$. To get the necessary condition, we only need to testify whether there is a unitary operator $V_1 = V'$ with parameters being $\varphi_1, \psi_1$ and $\chi_1$ as stated in Eq. (7) such that $P_{V_1}(\rho_V) = P_{V_1}(U)$. On the one hand, by Lemma 3, after calculation, we have

$$C_{33}\mathcal{V}_1(\rho) = \cos^2(2\varphi_1) + 2f_3 \sin^2(2\varphi_1) \sin^2(2\psi_1 + 2\chi_1) \quad (L4)$$

And on the other hand, by Lemma 4, we get

$$C_{33}\mathcal{V}_1(U) = \cos^2(2\varphi_1) \quad (L5)$$

Thus by $C_{33}\mathcal{V}_1(\rho) = C_{33}\mathcal{V}_1(U), 2f_3 \sin^2(2\varphi_1) \sin^2(2\psi_1 + 2\chi_1)$ should be 0. Since $\sin^2(2\varphi_1) \neq 0 (P \neq (0, 0, 1))$, we get $\sin(2\psi_1 + 2\chi_1) = 0$ or $f_3 = 0$. Then, by $V_1 = V'$, $\varphi_1 = \varphi, \psi_1 = -\psi$ and $\chi_1 = \chi + \pi$. Thus, finally we get the necessary condition is $f_2 = f_3 = 0$ or $f_2 = \sin(2\chi - 2\psi) = 0$.

**Appendix M: PROOF OF THEOREM 4**

**Proof.** Denote the new values of $P$ for $\rho$ and $U$ are $P_-(\rho)$ and $P_-(U)$. Obviously,

$$P_-(\rho) = P((V_- \otimes V_-)'\rho) = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}. \quad (M1)$$

The sum of the three entries of $P_-(\rho)$ is equal to -1, then $P_-(\rho)$ is in the plane $l(-1)$. For $P_-(U)$, we first prove $P_-(U) = P(V_-^tUV_-).$ Supposing $\xi$ is one of the two spectral measures associated with an observable $\sigma_i (i = 1, 2, 3)$, we measure the qubit before and after unitary operation $U$. The probability that the outcome of the measurement before unitary operation $U$ is $V_-|\xi_i\rangle$ and the outcome of the measurement after unitary operation $U$ is $V_+|\xi_i\rangle$ is

$$|\xi_i|V_-^tU^tV_+|\xi_i\rangle \langle \xi_i |V_-^tUV_-|\xi_i\rangle \quad (M2)$$

where after the first measurement, the state of the qubit collapsed to $V_-|\xi_i\rangle$. According to Eq. (M2), $V_-^tUV_-$ can be seen as a new $U$, then we get $P_-(U) = P(V_-^tUV_-)$. By Lemma 2 and Lemma 4, a straightforward computation can soon gives

$$P_-(U) = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}. \quad (M3)$$

It is also in the plane $l(-1)$.

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