Quantum Causal Inference in the Presence of Hidden Common Causes: an Entropic Approach

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Abstract

Quantum causality is an emerging field of study which has the potential to greatly advance our understanding of quantum systems. One of the most important problems in quantum causality is linked to this prominent aphorism that states correlation does not mean causation. A direct generalization of the existing causal inference techniques to the quantum domain is not possible due to superposition and entanglement. We put forth a new theoretical framework for merging quantum information science and causal inference by exploiting entropic principles. For this purpose, we leverage the concept of conditional density matrices to develop a scalable algorithmic approach for inferring causality in the presence of latent confounders (common causes) in quantum systems. We apply our proposed framework to an experimentally relevant scenario of identifying message senders on quantum noisy links, where it is validated that the input before noise as a latent confounder is the cause of the noisy outputs. We also demonstrate that the proposed approach outperforms the results of classical causal inference even when the variables are classical by exploiting quantum dependence between variables through density matrices rather than joint probability distributions. Thus, the proposed approach unifies classical and quantum causal inference in a principled way. This successful inference on a synthetic quantum dataset can lay the foundations of identifying originators of malicious activity on future multi-node quantum networks.

Keywords: Structure learning, Confounder, Common Cause, Optimization, Quantum causality

1. Introduction

Causal inference lies at the heart of science (Pearl, 2009; Pearl and Mackenzie, 2018): the conclusions drawn from scientific studies almost always involve extracting causation (cause and effect relationships) from association, even if researchers often refrain from explicitly acknowledging the causal goal of research projects (Hernán, 2018; Hernán et al., 2019). However, causal inference from observational data is an ambitious and difficult task. Identifying cause and effect relationships from observational data is even more challenging in the presence of hidden common causes (latent confounders) (Heckerman, 2019). The broad impact of this phenomena has been studied in multiple domains of science such as epidemiologic studies (Lipsitch et al., 2010), biology and medicine (Skelly et al., 2012; Meinshausen et al., 2016), experiential education (Ewert and Sibthorp, 2009; Kallus et al., 2018), economics and marketing (Varian, 2016; Hünermund and Bareinboim, 2019), among others.

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A similar concept is increasingly appreciated among quantum physicists, namely the inference of quantum common causes (Wolfe et al., 2020; Allen et al., 2017; Ried et al., 2015; Chaves et al., 2014a,b, 2015; Hofer-Szabó et al., 1999). It has been used to provide a satisfactory causal explanation (i.e., non-fine-tuned) of Bell inequality violations (Allen et al., 2017; Hofer-Szabó et al., 1999). This also has led to a formalization of quantum causal models (Costa and Shrapnel, 2016; Barrett et al., 2019; Chiribella and Ebler, 2019; Shrapnel, 2019). As shown in (Chaves et al., 2014a,b, 2015), in some cases, (hidden) common causes can be distinguished from direct causation using information theoretical generalization of Bell's inequalities and causal directed acyclic graphs (DAGs). Also, as shown in (Fitzsimons et al., 2015; Ried et al., 2015), observed quantum correlations alone are sometimes enough to imply causation. However, the proposed approach in (Fitzsimons et al., 2015; Ried et al., 2015) depends on the precise knowledge of the physical system and the measurement apparatuses (Gachechiladze et al., 2020). In this paper, we propose the first tractable algorithmic approach to distinguish between a hidden common cause and direct causal influences among two observed quantum systems without any interventional data.

To show the difficulty of causal structure discovery task even in the simplest classical case, where our observation consists of only two jointly-distributed random variables X and Y that are statically correlated, we recall Reichenbach's common cause principle (Reichenbach, 1991): If two random variables X and Y are statistically dependent, then there exists a third variable Z that causally affects both. As a special case, Z may coincide with either X or Y. Furthermore, this variable Z makes X and Y conditionally independent, i.e., $X \perp \!\!\!\perp Y | Z$. So, possible candidates for representing causal relationships between X and Y are: $X \to Y$, $X \leftarrow Y$, and $X \leftarrow Z \to Y$, and there is no easy way to determine which one is the right structure based on the observational data alone. The variable Z in the case $X \leftarrow Z \to Y$ is called unmeasured (latent) confounder or unmeasured (latent) common cause. So, one of the fundamental questions in causality is to determine how cause-effect relationships can be inferred from statistical information, encoded as a joint probability distribution, obtained under normal, intervention-free experiments.

To discover the true cause-effect relationships, scientists normally perform randomized experiments where a sample of units drawn from the population of interest is subjected to the specified manipulation directly. In many cases, however, such a direct approach is not possible due to expense or ethical considerations. Instead, investigators have to rely on observational studies to infer causality. This task is even more challenging in quantum context due to quantum superpositions and entanglement relations. In this work, we are interested in quantum generalizations of causal structures in the presence of latent common causes. These structures can be shown as a directed acyclic graph (DAG), where nodes are quantum systems, and edges are quantum operations¹. However, the key theoretical distinction between an entirely classical causal structure and a quantum casual structure is the concept of coexisting. Because of the impossibility of cloning, the outcomes and the quantum systems that led to them do not exist simultaneously. If a system X is measured to produce Y, then ρ_{XY} is not defined and hence neither is the entropy $S(\rho_{XY})$ (Weilenmann and Colbeck, 2017). For a given causal structure, a coexisting set of systems is one for which

^{1.} In the context of quantum computation (Hogg, 1996), a quantum operation is called a quantum channel.

a joint state can be defined (Chaves et al., 2015; Weilenmann and Colbeck, 2017, 2020). If we pick a coexisting set of nodes (e.g., a classical system, or a set of nodes that are created at the same instance of time, i.e., they do enjoy a joint density operator), then we can investigate the identification of quantum causal structures in the presence of latent confounders.

In this paper, we consider causality between two coexisting quantum subsystems. As a part of the evaluation framework, we provide a model of such a coexisting system, where two entangled qubits are used, and one of the qubit is transmitted over a quantum channel. Similarly, three entangled qubits are used, and two of them are transmitted over two separate quantum channels. The models can be further generalized, while note that the subsystems which are being considered for quantum causality relationships have to coexist, unlike in the classical case where it is not necessary for the sub-systems

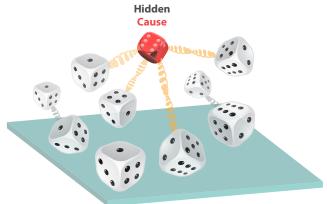


Figure 1: We develop a theoretical framework for solving the problem of quantum common cause.

to coexist. To address this problem, we introduce a theoretical framework to merge quantum information science with causal inference using entropic principles. Classically, it has been proposed and tested that minimization of the trade-off between the entropy of the (hidden) common cause Z (i.e., H(Z)) and the conditional mutual information of observed variables X and Y given Z (i.e., I(X;Y|Z)) can be used to distinguish the latent graph $X \leftarrow Z \rightarrow Y$ (Z is an unmeasured confounder) from the directed graphs $X \rightarrow Y$ and $X \leftarrow Y$ based on observational data alone under certain assumptions (Kocaoglu et al., 2020) (a brief review is given in Section 2). We will provide the first generalization of this approach to the quantum domain (Figure 1).

Even though the paper considers an approach for quantum causal inference, we also apply the proposed approach to a classical setup, where two bits are transmitted over a binary symmetric channel (to illustrate the case of no confounder), or two bits are transmitted over two separate channels (to illustrate the case of latent confounder). We show that the proposed approach outperforms the classical causal inference in (Kocaoglu et al., 2020) due to the use of quantum density matrix. We note that finding the optima over a quantum density matrix rather than over the probability distribution function provides larger degrees of freedom thus resulting in improved results. This demonstrates that the proposed approach can also be used for classical causal inference with improved results. Our main contributions are as follows:

- Inferring causality in the presence of latent confounders from observational data alone is one of the most important and challenging problems in statistical inference. We propose an iterative algorithm, called QInferGraph, for identifying *latent confounders* in Section 3. Our method leverages the concept of quantum conditional matrices to unify the solution for classical and quantum (latent) common cause problem in a principled way.
- We evaluate the proposed approach for classical causal inference. By leveraging optimiza-

tion over density matrices, the proposed approach is shown to outperform the results of classical causal inference in (Kocaoglu et al., 2020).

• We put forth an experimental scheme that can be used to confront our theoretical framework. We consider a minimalistic model of an unknown message (possibly encrypted) with unknown origin in a two-node quantum network with the possibility of the presence of a latent common cause, where nodes are a coexisting set of quantum systems for which a joint density matrix can be defined. Entangled quantum subsystems are used, where subsystems are communicated over noisy channels (e.g., optical fiber) to create such coexisting set of quantum systems. We prove that only using the joint density matrix of the observed two quantum system, we can identify the originator of the message (i.e., the sub-system that did not encounter the noisy channel). To verify the validation of QInferGraph, we use realistic quantum noisy links such as quantum symmetric channel and depolarizing channel (valid for quantum networking and quantum communications) (Section 4). Moreover, we show that finding the joint probability distribution and using the classical common entropy technique may result in erroneous outcomes, as shown in Section 5, thus showing that the classical approaches cannot be directly used on quantum systems. This specific approach can lay the foundations of identifying originators of malicious activity on multi-node quantum networks.

The rest of the paper is organized as follows. In Section 2, we review the classical causal inference approach proposed in (Kocaoglu et al., 2020) for the identification of causal structures in the presence of hidden common causes. In Section 3, we generalized the classical approach to the quantum domain. In Section 4, we put forward an experimental scheme that can be used to validate our proposed approach using a minimalistic model of an unknown message (possibly encrypted) with unknown origin in a two-node/three-node quantum network. In Section 5, we explain and show why should we not map quantum to classical directly. In Appendix A and B, we provide details on the best choice of hyper-parameters of our proposed algorithm.

2. Review of Classical Causal Inference Framework in (Kocaoglu et al., 2020)

In this section, we briefly review the proposed approach in (Kocaoglu et al., 2020) for confounder discovery via solving an optimization problem that its aim is to discover the trade-off between the entropy of the latent variable and the conditional mutual information of the observed variables. Consider that the joint distribution P(X,Y) between two observed variables is given. The goal is to find a random variable Z that makes X and Y conditionally independent given Z. Possible cases that can represent this situation is shown in Figure 2.

In the classical causal inference, Kocaoglu et al. (2020) distinguished between *latent* graph in Figure 2(a) from others in Figure 2 based on unmeasured confounder having low Shannon entropy under certain assumptions. Formally, the following was assumed:

Assumption 1 Consider any causal model with observed variables X and Y. Let Z represents the variable that captures all latent confounders between X and Y. Then $H(Z) < \theta$, where $H(Z) = -\sum_{i=1}^{n} P(x_i) \log(x_i)$.

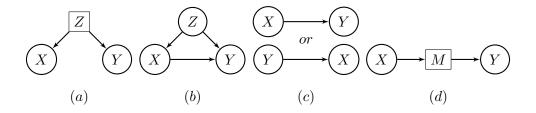


Figure 2: (a) Latent Graph, (b) Triangle Graph, (c) Direct Graph, and (d) Mediator Graph.

```
Algorithm 1: LatentSearch (Kocaoglu et al., 2020)

Input: Supports of X, Y, and Z, respectively; Joint probability distribution p(x, y); Number of iterations N; \beta in the loss function L = I(X;Y|Z) + \beta H(Z), Initialization of q_1(z|x,y).

Output: Joint distribution q(x,y,z).

1 for i=1:N do

/* Form the joint distribution:

q_i(x,y,z) \leftarrow q_i(z|x,y)p(x,y), \forall x,y,z;

Calculate:

q_i(z|x) \leftarrow \frac{\sum_{y \in Y} q_i(x,y,z)}{\sum_{y \in Y,z \in Z} q_i(x,y,z)}, q_i(z|y) \leftarrow \frac{\sum_{x \in X} q_i(x,y,z)}{\sum_{x \in X,z \in Z} q_i(x,y,z)}, q_i(z) \leftarrow \sum_{x \in X,y \in Y} q_i(x,y,z)

4 Update:

q_{i+1}(z|x,y) \leftarrow \frac{1}{F(x,y)} \frac{q_i(z|x)q_i(z|y)}{q_i(z)^{1-\beta}}, \text{ where } F(x,y) = \sum_{z \in Z} \frac{q_i(z|x)q_i(z|y)}{q_i(z)^{1-\beta}}

5 end

6 return q(x,y,z) := q_{N+1}(z|x,y)p(x,y).
```

Assumption 2 Consider a causal model where X causes Y. If X causes Y only through a latent mediator Z, i.e., $X \to Z \to Y$, then $H(Z) \ge \theta$.

Note that I(X;Y|Z)=0 means that Z makes the variables X and Y conditionally independent, i.e., $X \perp \!\!\! \perp Y|Z$. To identify latent graphs, Kocaoglu et al. (2020) proposed an iterative algorithm (Algorithm 1) that discovers the trade-off between the entropy of the unmeasured confounder and the conditional mutual information of the observed variables. This trade-off is formally defined as follows:

$$L = I(X; Y|Z) + \beta H(Z) \tag{1}$$

In fact, **LatentSearch** (Algorithm 1) sets q(x, y, z) = q(z|x, y)p(x, y) and searches over q(z|x, y) to find the stationary point of the loss function L in Equation (1). For this purpose, **LatentSearch** returns a joint probability distribution q(X, Y, Z) from which the Shannon entropy of the latent variable W, i.e., H(W) can be computed. To verify whether the causal graph $G = (V = \{X, Y\}, E)$ is a latent graph or not, **InferGraph** (Algorithm 2) (Kocaoglu et al., 2020) runs **LatentSearch** multiple times and selects the smallest H(W)

^{2.} Note that this is different from the notion of *causal independence*, which refers to the situation where multiple causes contribute independently to a common effect (Zhang and Poole, 1996).

discovered by the algorithm among those that ensure the conditional independence of X and Y given W, i.e., $I(X;Y|W) \leq \theta$ for a practical threshold (as suggested in (Kocaoglu et al., 2020), $\theta = 0.001$). We refer readers to (Kocaoglu et al., 2020) for more experimental settings. Kocaoglu et al. (2020) conjecture that, under assumptions 1, 2 and in practice, the Shannon entropy of observed variables X and Y for directed graphs and triangle graphs is lower-bounded by the entropies of X and Y, up to a scaling by a constant (as suggested in (Kocaoglu et al., 2020), $0.8 \min\{H(X), H(Y)\}$). For more detailed discussion see (Kocaoglu et al., 2020).

Algorithm 2: InferGraph: Identifying the Latent Graph (Kocaoglu et al., 2020)

```
Input: Joint probability distribution p(x,y); Number of iterations N; I(X;Y|Z) threshold T; H(Z)
            threshold that is determined by \theta = \alpha \min(H(X), H(Y)); \{\beta_i\}_{i=1}^N; Support size of X, Y, and Z,
            i.e., r, m, and n, respectively.
    Output: "Latent Graph" if Z is an unmeasured confounder for X and Y, otherwise, returns "Triangle or
               Direct Graph".
 1 for i = 1 : N do
        q_i(x, y, z) \leftarrow \mathbf{LatentSearch}(p(x, y), \alpha, \beta_i, r, m, n);
        Calculate I_i(X;Y|Z) and H_i(Z) from q_i(x,y,z);
 3
 4 end
 5 S = \{i : I_i(X; Y|Z) \le T\};
 6 if \min(H_i(Z): i \in S) > \theta or S = \emptyset then
        return Triangle or Direct Graph;
 8 else
 9
        return Latent Graph;
10 end
```

3. Proposed Entropic Approach for Confounder Discovery in Quantum Systems

In this section, we provide an approach for identifying latent graphs in quantum systems, where we assume the Assumptions 1 and 2, with the entropy replaced by the von-Neumann entropy, $S(X) = -\text{tr}(\rho_X \log \rho_X)$. We first briefly review the formalism of quantum conditional density matrices, which provides a solid framework for adapting classical iterative algorithms (Algorithm 1 and 2) to the quantum domain. Then, the proposed algorithm to identify latent graphs is described which uses the concept of the quantum conditional density matrix.

3.1 Conditional Density Matrix

Quantum theory can be understood as a non-commutative generalization of classical probability theory wherein probability measures are replaced by density operators (Leifer and Spekkens, 2013). Analogies between the classical theory of Bayesian inference and the conditional states formalism for quantum theory are listed in Table 1.

Quantum conditional densities are a generalization of classical conditional probability distributions. However, to generalize conditional probabilities to the quantum case, several approaches have been proposed in the literature. The three following generalizations are the best known in the literature of quantum information: (1) quantum conditional expectation (Umegaki, 1962), (2) quantum conditional amplitude operator (Cerf and Adami, 1997, 1999), and (3) quantum conditional states (Leifer, 2007; Leifer and Spekkens, 2013).

Classical Probability	Quantum Theory
probability distribution $p(X)$	density operator (matrix) ρ_X
joint distribution $p(X,Y)$	joint density ρ_{XY}
marginal distribution $p(X) = \sum_{Y} p(X, Y)$	partial trace $\rho_X = Tr_Y(\rho_{XY})$
conditional probability	conditional density (Leifer, 2007; Leifer and Spekkens, 2013)
p(X Y) = p(X,Y)/p(Y)	$\rho_{X Y} = (I_X \otimes \rho_Y^{-1/2}) \rho_{XY} (I_X \otimes \rho_Y^{-1/2})$
instance conditional probability	instance conditional density matrix (Javidian et al., 2021)
$p(X Y = y) = \frac{p(X,Y=y)}{\sum_{x} p(X,Y=y)}$	$ \rho_{X Y= y\rangle} = \frac{Tr_Y\{\rho_{XY}\star y\rangle\langle y \}}{trace\{Tr_Y\{\rho_{XY}\star y\rangle\langle y \}\}}, \text{ where} $
	$\rho_{XY} \star y\rangle\langle y = (I \otimes (y\rangle\langle y)^{1/2}) * \rho_{XY} * (I \otimes (y\rangle\langle y)^{1/2})$

Table 1: Analogies between classical and quantum formalism

Arguably, quantum conditional states are the most useful generalization of conditional probability from the point of view of practical applications. For example, quantum conditional states have been used in (Leifer and Spekkens, 2013) to build a quantum theory of Bayesian inference. Since quantum conditional states provides a closer analogy between quantum theory and classical probability theory, we choose this formalism to define quantum conditional density matrices. We will see that this formalism plays a significant role in the design and success of our entropic quantum causal inference algorithm.

3.2 QLatentSearch: An Algorithm for Computing Exact Quantum Common Entropy

In this section, we propose an iterative algorithm (Algorithm 3) that discovers the trade-off between the entropy of the unmeasured confounder and the quantum conditional mutual information of two observed quantum systems given the unmeasured confounder, which is fundamental for designing an algorithm for the identification of latent confounders in quantum systems as we show in the next subsection. This trade-off is formally defined as follows:

$$L = I_O(X; Y|Z) + \beta S(Z) \tag{2}$$

Note that $I_Q(X;Y|Z)=0$ implies that the quantum conditional independence of X and Y given Z (Allen et al., 2017, Theorem 3). Having low von Neumann entropy of hidden common cause Z, i.e., S(Z) under the quantum version of Assumption 1 and 2 enable us to identify latent graphs from direct/mediator graphs in practice, as we show in Section 4. For this purpose, rather than searching over ρ_{XYZ} and enforcing the constraint $\rho_{XY}=Tr_Z(\rho_{XYZ})$, we can search over $\rho(Z|X,Y)$ and set $\rho_{XYZ}=(\rho_{XY}^{-1/2}\otimes I_Z)\rho(Z|X,Y)(\rho_{XY}^{-1/2}\otimes I_Z)$ because:

$$\begin{split} L &= I_Q(X;Y|Z) + \beta S(Z) \\ &= S(XZ) + S(YZ) - S(Z) - S(XYZ) + \beta S(Z) \\ &= S(XZ) + S(YZ) - S(XYZ) + (\beta - 1)S(Z) \\ &= S(X) + S(Z|X) + S(Y) + S(Z|Y) - S(XY) - S(Z|X,Y) + (\beta - 1)S(Z) \\ &= S(Z|X) + S(Z|Y) - S(Z|X,Y) + (\beta - 1)S(Z) + I_Q(X;Y) \end{split}$$

Note that
$$\rho(Z|Y) = Tr_X((\rho^{1/2}(X|Y) \otimes I_Z)\rho(Z|X,Y)(\rho^{1/2}(X|Y) \otimes I_Z)), \ \rho(Z|X) = Tr_Y((\rho^{1/2}(Y|X) \otimes I_Z)\rho(Z|X,Y)(\rho^{1/2}(Y|X) \otimes I_Z)), \ \text{and} \ \rho_Z = Tr_{X,Y}((\rho_{XY}^{1/2} \otimes I_Z)\rho(Z|X,Y)(\rho_{XY}^{1/2} \otimes I_Z)\rho(Z|X,Y)(\rho_{XY}^{1/2} \otimes I_Z))$$

 I_Z)). So, we have $L = L(\rho(Z|X,Y))$, which is the counterpart of the classical loss function in Equation 1 with the following differences: (i) rather than using (conditional) probability distributions, we use (conditional) density matrices, and (ii) rather than using Rényi entropy, we use the von Neumann entropy.

We aim to optimize the objective L over $\rho(Z|X,Y)$. Although first order methods (e.g., gradient descent) or genetic algorithm (GA), which is a metaheuristic method inspired by the process of natural selection, can be used to find a stationary point of the optimization problem in (2), as we empirically observe the convergence is unattainable/slow and the performance is very sensitive to the tuning parameters such as step size and the mutation probability. This optimization problem is difficult to perform numerically because the boundary of the space of positive semidefinite matrices is hard to compute. In order to provide a scalable algorithm for this optimization, we extend the iterative algorithm that was proposed for classical version of the problem in (Kocaoglu et al., 2020).

The proposed iterative algorithm for the optimization of L is described in Algorithm 3, and is called QLatentSearch. This algorithm starts from a random initialization $\rho_1(Z|X,Y)$, and then at each iteration i does the following two phases to update $\rho_{i+1}(Z|X,Y)$ from $\rho_i(Z|X,Y)$ to finally minimize the loss function L in (2):

- Calculate Phase: In this phase we use partial trace to get $\rho_i(Z|X)$ (line 3-5), $\rho_i(Z|Y)$ (line 6-8), and ρ_Z^i (line 9) from ρ_{XYZ}^i .
- Update Phase: In this phase we update $\rho_{i+1}(Z|X,Y)$ to get ρ_{XYZ}^{i+1} (line 10) for the next iteration.

Algorithm 3: QLatentSearch, An Iterative Algorithm for Computing Exact Quantum Common Entropy

```
Input: Joint density matrix \rho_{XY}; Number of iterations N; \beta parameter in the loss function
                    L = I_Q(X; Y|Z) + \beta S(Z), Initialization of \rho_1(Z|X,Y).
      Output: Joint density matrix \rho_{XYZ}.
  1 for i = 1 : N do
             /* Form the joint density matrix: \rho^i_{XYZ} = (\rho^{1/2}_{XY} \otimes I_Z) \rho_i(Z|X,Y) (\rho^{1/2}_{XY} \otimes I_Z); \\ \text{/* Calculate Phase:}
                                                                                                                                                                                   */
             /* (i) Calculate \rho_i(Z|X):

ho_{XZ}^i=Tr_Y(
ho_{XYZ}^i) // Then, compute 
ho_{XI_YZ}^i by reordering the entries of 
ho_{XZ}^i
  3

\rho_X^{i} = Tr_Z(\rho_{XZ}^{i}); 

\rho_i(Z|X) \leftarrow ((\rho_X^{i})^{-1/2} \otimes I_{YZ})\rho_{XI_{YZ}}^{i}((\rho_X^{i})^{-1/2} \otimes I_{YZ});

             /* (ii) Calculate \rho_i(Z|Y):
                                                                                                                                                                                   */
             \rho^i_{YZ} = Tr_X(\rho^i_{XYZ}) // Then, compute \rho^i_{I_XYZ} = I_X \otimes \rho^i_{YZ}
             \rho_Y^i = Tr_Z(\rho_{YZ}^i);
             \rho_i(Z|Y) \leftarrow (I_X \otimes (\rho_Y^i)^{-1/2} \otimes I_Z) \rho_{I_X Y Z}^i(I_X \otimes (\rho_Y^i)^{-1/2} \otimes I_Z);
              /* (iii) Calculate 
ho_Z^i:
                                                                                                                                                                                    */
             \begin{array}{l} \rho_Z^i = Tr_{XY}(\rho_{XYZ}^i);\\ \text{/* Update Phase:} \end{array}
                                                                                                                                                                                    */
             \rho_{i+1}(Z|X,Y) \leftarrow (I_{XY} \otimes (\rho_Z^i)^{\beta-1})\rho_i(Z|X)\rho_i(Z|Y);
10
12 return \rho_{XYZ} := (\rho_{XY}^{1/2} \otimes I_Z) \rho_{N+1}(Z|X,Y) (\rho_{XY}^{1/2} \otimes I_Z).
```

3.3 QInferGraph: An Algorithm for the Identification of Latent Confounders

In this section, we propose a quantum entropic approach to causal inference that can discern the difference between causation and correlation. Specifically, under the assumption that there are no low-entropy mediators (Assumption 2), Algorithm 3 can be used to distinguish causation from spurious correlation between two observed quantum systems. This enables us to distinguish latent graph in Figure 2(a) from the triangle or direct graphs in Figure 2(b)-(c). Our main assumption is that the latent confounders, if they exist, have small von Neumann entropy. In other words, in Figure 2(a), $S(Z) \leq \theta$ for some θ . Similar to the classical version of this problem, we conjecture that $\theta = \alpha \min\{S(X), S(Y)\}$ for some $\alpha < 1$. Considering Assumption 1 and Assumption 2 along with QLatentSearch (Algorithm 3), we propose an algorithm, called QInferGraph (Algorithm 4), to identify latent graphs.

Algorithm 4: QInferGraph: Identifying the Latent Graph

```
Input: Joint density matrix \rho_{XY}; Number of iterations N; I_Q(X;Y|Z) threshold T; S(Z) threshold that
             is determined by \theta = \alpha \min(S(X), S(Y)); \{\beta_i\}_{i=1}^N. The number of rows (or equivalently, columns)
             of X, Y, and Z, i.e., r, m, and n, respectively.
    Output: "Latent Graph" if Z is an unmeasured confounder for X and Y, otherwise, returns "Triangle or
               Direct Graph".
 1 for i = 1 : N do
         \rho_{XYZ}^{i} \leftarrow \mathtt{QLatentSearch}(\rho_{XY}, \alpha, \beta_{i}, r, m, n);
         Calculate I_Q^i(X;Y|Z) and S_i(Z) from \rho_{XYZ}^i;
 3
 4
    end
 5 S = \{i : I_O^i(X; Y|Z) \le T\};
 6 if \min(S_i(Z): i \in S) > \theta or S = \emptyset then
         return Triangle or Direct Graph;
    else
        return Latent Graph;
10 end
```

In short, QInferGraph calls QLatentSearch N times to figure out if there exist a W, for which $I_Q(X;Y|W) < T$, i.e., W makes X and Y conditionally independent. Also, the von Neumann entropy of W is enough small such that $S(W) < \alpha \min\{S(X), S(Y)\}$ for some α in practice. If there exist such a W, the algorithm declares W is a latent confounder. In other words, latent graph represents correlation without causation relationship between observed quantum systems X and Y. Otherwise, very likely such a W that minimizes the loss function L does not exist, and QInferGraph declares that a triangle graph or a direct graph represents the connection between X and Y better than a latent graph in this case. In the next section we conduct experiments to verify this procedure in practice.

4. Evaluation on Quantum Causal Synthetic Data

Since there is no quantum cause-effect repository to verify the validity of our proposed algorithm, we put forward an experimental scheme that can be used to confront our theoretical framework. To show the effectiveness of the proposed approach in section 3, we use quantum noisy links, where it is validated that the input before noise, as a latent confounder (hidden source), is the cause of the noisy outputs, as shown in Figure 3.

We first apply the proposed approach to a classical setup, as explained in Model 1, where two bits are transmitted over a binary symmetric channel (to illustrate the case of no



Figure 3: Alice and Bob are connected by a noisy channel (e.g., an optical fiber) with an unknown source of message.

confounder), or two bits are transmitted over two separate channels (to illustrate the case of latent confounder). We show that the proposed approach outperforms the classical causal inference in (Kocaoglu et al., 2020) due to the use of quantum density matrix. Finding the optima over a quantum density matrix rather than over a probability distribution provides larger degrees of freedom thus resulting in improved results. Our results indicate that the proposed approach can also be used for classical causal inference with improved results.

Model 1 (Classical Binary Symmetric Channel: Latent and Direct Graph) Part I: Latent Graph. Assume a 2-bit input $Z \in \{00,01,10,11\}$. Let each bit of Z be in the state 1 with probability q and 1-q otherwise, and independent of each other. So, $p(Z=00)=(1-q)^2$, p(Z=01)=p(Z=10)=q(1-q), and $p(Z=11)=q^2$. Z is transmitted over a binary symmetric channel with independent bit error probability of p_1 , and is denoted X. A cloned version of Z is transmitted over a binary symmetric channel with independent bit error probability of p_2 , and is denoted Y. The joint probability distribution of X,Y, and Z, where Z is the cause of X and Y, i.e., $X \leftarrow Z \rightarrow Y$ can be computed as p(X,Y,Z)=p(Z)p(X|Z)p(y|Z). For example, $p(01,10,00)=(1-q)q*p_1p_2*(1-p_1)p_2$. Then we marginalize out Z to obtain the joint probability distribution for the latent graph $X \leftrightarrow Y$. Note that the corresponding joint density matrix ρ_{XY} is a diagonal matrix that its diagonal entries come from the joint probability distribution p(X,Y). The key reason of constructing ρ_{XY} as the diagonal matrix from p(X,Y) is to have the mixed states, so that the von-Neuman entropy of ρ_{XY} is the same as the Shannon entropy of p(X,Y).

Now, we apply QInferGraph (Algorithm 4) on ρ_{XY} to verify that X and Y are confounded by Z. For this purpose, we use QLatentSearch (Algorithm 3) on 100 different values of β , uniformly spaced in the interval (0.7,0.8). A discussion regarding the best choice of β can be found in appendices A and B. We run QLatentSearch for 500 iterations each time. We use the conditional mutual information threshold of 0.05. In other words, of the algorithm outputs for the 100 β values used, we pick the smallest entropy W discovered by the algorithm among those that ensure $I(X;Y|W) \leq 0.05$. Table 9 summarizes the results for different S(W) threshold that is determined by $\theta = \alpha \min\{S(X), S(Y)\}$. For different values of $\alpha = 0.7, 0.8, 0.9, 1$, the results are the same, and are given in Table 2. We let q = 0.4. In the Table, T means that QInferGraph (Algorithm 4) identifies the latent

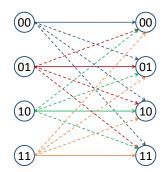


Figure 4: 2-bit non-Binary symmetric channel.

Table 2: Validation of Latent Graph in Model 1 (Part I) for $\alpha = 0.7, 0.8, 0.9, 1$, and $\beta \in (0.7, 0.8)$ via QInferGraph.

						p_2	2					
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
	0.01	F	\mathbf{F}	F	F	T	T	T	\mathbf{F}	\mathbf{F}	F	\mathbf{F}
	0.1	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{F}
	0.2	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{F}	\mathbf{F}	\mathbf{F}
	0.3	\mathbf{F}	\mathbf{T}	\mathbf{F}								
	0.4	\mathbf{T}										
p_1	0.5	\mathbf{T}										
	0.6	\mathbf{T}										
	0.7	\mathbf{F}	\mathbf{T}	${ m T}$	\mathbf{T}	\mathbf{F}						
	0.8	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{F}	\mathbf{F}	\mathbf{F}
	0.9	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{F}	${f T}$	${f T}$	\mathbf{T}	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{F}
	0.99	F	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{F}	\mathbf{F}	\mathbf{F}	F

graph correctly. But, \mathbf{F} means that the algorithm fails to identify the latent graph. For very small or very large p_i 's the case of latent confounder or direct graph are hard to separate, while the proposed algorithm works well in most other cases.

Now, if we apply **InferGraph** (Algorithm 2) on p(X,Y) with $\alpha=0.8$, as suggested in (Kocaoglu et al., 2020), and two different β parameters: (1) the same as one that we used in Table 2 in QInferGraph, i.e., $\beta \in (0.7,0.8)$, and (2) the same as one that suggested in (Kocaoglu et al., 2020), i.e., $\beta \in (0,0.1)$, we obtain the results summarized in Table 3.

Some highlights for results in Part I: (1) Note that where the probability of errors i.e., p_1 and p_2 are very small, the latent confounder Z is hardly distinguishable from X (or Y) and QInferGraph fails to discover the latent graph. (2) Note that QLatentSearch tries to find the stationary point(s) of the loss function L in Equation (2), and there is no guarantee to find the global optimum. However, the performance of QInferGraph in this case is acceptable: true positive rate (recall) = 0.6, false positive rate (fall-out) = 0, false negative rate (miss rate) = 0.4, accuracy = 0.6. (3) The hyperparameter α does not affect significantly on the quality of results in our experimental settings that indicates QInferGraph is not very sensitive to hyperparameters. (4) Although InferGraph (Algorithm 2) perfectly identifies

Table 3: Validation of Latent Graph in Model 1 (Part I) via classical causal inference (Algorithm 2), and $\alpha = 0.8$.

				(a) β	$\in (0$	0, 0.	1)									(b)	$\beta \in$	€ (0	.7, 0	.8)				
						p_2	2												p_{z}	2					
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99			0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
	0.01	T	T	T	T	T	T	T	T	T	T	T		0.01	T	F	F	F	F	T	F	F	F	F	T
	0.1	T	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	T	\mathbf{T}	T	\mathbf{T}	\mathbf{T}	\mathbf{T}		0.1	F	\mathbf{F}	\mathbf{F}	\mathbf{F}	F	T	F	F	\mathbf{F}	F	F
	0.2	T	\mathbf{T}	\mathbf{T}	T	T	T	T	T	T	T	\mathbf{T}		0.2	F	F	F	F	F	T	F	\mathbf{F}	\mathbf{F}	\mathbf{F}	F
	0.3	T	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	T	T	T	T	\mathbf{T}	\mathbf{T}		0.3	F	F	F	\mathbf{F}	F	T	F	\mathbf{F}	\mathbf{F}	\mathbf{F}	F
	0.4	T	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	T	\mathbf{T}	T	\mathbf{T}	\mathbf{T}	\mathbf{T}		0.4	F	\mathbf{F}	\mathbf{F}	\mathbf{F}	F	T	F	F	\mathbf{F}	F	F
p_1	0.5	T	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	T	\mathbf{T}	T	\mathbf{T}	\mathbf{T}	\mathbf{T}	p_1	0.5	T	\mathbf{T}	\mathbf{T}	T	\mathbf{T}	T	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	T
	0.6	T	\mathbf{T}	\mathbf{T}	T	T	T	T	T	T	T	\mathbf{T}		0.6	F	F	F	F	F	T	F	\mathbf{F}	\mathbf{F}	\mathbf{F}	F
	0.7	T	\mathbf{T}	\mathbf{T}	T	T	T	T	T	T	T	\mathbf{T}		0.7	F	F	F	F	F	T	F	\mathbf{F}	\mathbf{F}	\mathbf{F}	F
	0.8	T	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	T	T	T	T	\mathbf{T}	\mathbf{T}		0.8	F	F	F	\mathbf{F}	F	T	F	\mathbf{F}	\mathbf{F}	\mathbf{F}	F
	0.9	T	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	T	\mathbf{T}	T	\mathbf{T}	\mathbf{T}	\mathbf{T}		0.9	F	\mathbf{F}	\mathbf{F}	\mathbf{F}	F	T	F	F	\mathbf{F}	F	F
	0.99	T	T	T	T	T	T	T	T	T	T	T		0.99	T	F	F	F	F	T	F	F	F	F	T

latent graphs in Model 1 (Part I), it fails to identify latent graphs in many cases (about 80%). (5) It seems that the classical causal inference algorithm, i.e., **InferGraph** (Algorithm 2) outperforms QInferGraph in classical data. However, as we will see in Part II of Model 1, the performance of the classical algorithm is not consistent (no longer outperform QInferGraph), where there is no latent confounder.

Part II: Direct Graph. Assume that there is a 2-bit symmetric noisy channel, where there is no latent common cause, i.e., there is an input X and an output Y, as shown in Figure 4, with the same properties explained in Part I. The results of applying QInferGraph and InferGraph on p(X,Y) and ρ_{XY} are summarized in Table 4 and 5, respectively. T means that QInferGraph (Algorithm 4) identifies the direct graph correctly. But, F means that the algorithm fails to identify the direct graph.

Table 4: Validation of Direct Graph in Model 1 (Part II) via QInferGraph.

						p						
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
	0.7	${f T}$	T	T	T	F	T	F	T	T	T	\mathbf{T}
	0.8	${f T}$							\mathbf{T}			
α	0.9	${f T}$	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{F}	\mathbf{T}	\mathbf{F}	${f T}$	\mathbf{T}	\mathbf{T}	${f T}$
	1	\mathbf{T}	T	T	\mathbf{T}	\mathbf{F}	\mathbf{T}	\mathbf{F}	T	\mathbf{T}	\mathbf{T}	\mathbf{T}

Table 5: Validation of Latent Graph in Model 1 (Part II) via classical causal inference (Algorithm 2).

		(a) $\beta \in (0, 0.1)$ $\begin{array}{c ccccccccccccccccccccccccccccccccccc$												(b) β	€ (0).7,(0.8)							
						p	,												p	,					
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99			0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
	0.7	T	T	T	F	F	T	F	F	T	T	T		0.7	F	T	T	T	T	T	T	T	T	T	F
	0.8	F	F	\mathbf{F}	F	F	\mathbf{T}	F	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{F}		0.8	F	T	\mathbf{T}	\mathbf{T}	T	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	F
α	0.9	F	F	F	F	F	\mathbf{T}	F	F	F	\mathbf{F}	\mathbf{F}	α	0.9	F	\mathbf{T}	\mathbf{F}								
	1	F	F	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{T}	\mathbf{F}	\mathbf{F}	F	\mathbf{F}	F		1	F	\mathbf{T}	T	\mathbf{T}	F						

Some highlights for results in Part II: (1) Note that when p = 0.5, X and Y are uncorrelated and then X and Y are not cause and effect. In this case, T means that both

quantum and classical algorithms identify that X and Y are not cause and effect, as we expected. (2) Although the performance of the classical algorithm (Algorithm 2), where $\beta \in (0,0.1)$, is perfect for Model 1 (Part I), its performance for Model 1 (Part II), where there is no confounder, is not acceptable.

In conclusion, results from Part I and II, indicate that QInferGraph is a more consistent and less sensitive to the change of parameters than its counterpart in the classical causal inference, even for the classical data.

Next, we apply our proposed approach on a quantum (non-classical) model, as explained in Model 2, where mixed entangled quantum subsystems are used for which subsystems are communicated over noisy channels (e.g., optical fiber) to create a coexisting set of quantum systems.

Model 2 (Depolarizing Quantum Channel: Latent Graph and Direct Graph) Part I: Latent Graph. Assume that there are real numbers γ_1 , γ_2 , λ_1 , and λ_2 such that $\gamma_1^2 + \lambda_1^2 = 1$ and $\gamma_2^2 + \lambda_2^2 = 1$. We consider a joint entangled system (of three qubits) as the mixture of the following pure density matrices:

```
\begin{cases} [(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)][(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)]^{\dagger} & q \\ [(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)][(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)]^{\dagger} & 1 - q \end{cases}
```

In other words, the system considered has density matrix $q[(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)[(\gamma_1|0\rangle + \lambda_1|1\rangle)(\gamma_1|0\rangle + \lambda_1|1\rangle)]^{\dagger} + (1-q)[(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)[(\gamma_2|0\rangle + \lambda_2|1\rangle)(\gamma_2|0\rangle + \lambda_2|1\rangle)]^{\dagger}$. The system is a mixture of two pure density matrices. This quantum system has entanglement among the three quantum bits. Let the second quantum bit is transmitted over a quantum depolarizing channel with error probability p_1 , and the third quantum bit is transmitted over a quantum depolarizing channel with error probability p_2 . Note that the depolarizing channel with error probability p_1 has no error with probability p_2 . Note that the depolarizing channel with error probability p_1 has no error with probability p_2 . Note that the depolarizing channel with error probability p_1 has no error with probability p_2 . Note that p_1 is p_2 (Nielsen and Chuang, 2002). With this setup, the joint density matrix is given as $p_{ZXY} = q \rho_{ZXY}^{\gamma_1,\lambda_1} + (1-q) \rho_{ZXY}^{\gamma_2,\lambda_2}$, where $p_{ZXY}^{\gamma_2,\lambda_2}$ is given as the mixture of the following pure density matrices:

```
[(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)][(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (1-p_1)(1-p_2)
 [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)][(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (1-p_1)(p_2/3)
[(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)][(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (1-p_1)(p_2/3)
[(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)][(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (1-p_1)(p_2/3)
 [(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)[(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (p_1/3)(1-p_2)
 [(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)][(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (p_1/3)(p_2/3)
 [(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)][(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (p_1/3)(p_2/3)
 [(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)][(\gamma|0\rangle + \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (p_1/3)(p_2/3)
 [(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)[(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (p_1/3)(1-p_2)
 [(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)][(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (p_1/3)(p_2/3)
[(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)][(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (p_1/3)(p_2/3)
[(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)][(\gamma|0\rangle + \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (p_1/3)(p_2/3)
[(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)[(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(\gamma|0\rangle + \lambda|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (p_1/3)(1-p_2)
[(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)][(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(\lambda|0\rangle + \gamma|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (p_1/3)(p_2/3)
 [(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)][(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(-\lambda|0\rangle + \gamma|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (p_1/3)(p_2/3)
[(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)[(\gamma|0\rangle + \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)(\gamma|0\rangle - \lambda|1\rangle)]^{\dagger}
                                                                                                                                                                                                                                            (p_1/3)(p_2/3)
```

We note that X and Y coexist, thus we can find joint density matrix of X and Y by tracing out Z in ρ_{ZXY} . Then, we apply QInferGraph (Algorithm 4) on ρ_{XY} to verify that X and Y are confounded by a latent variable. For this purpose, we use the same parameters specification as explained in Model 3, and q=0.4. Table 6 summarizes the results for different entropy threshold of the latent confounder that is determined by $\theta=\alpha\min\{S(X),S(Y)\}$, where $\alpha=0.7,0.8,0.9,1$. T means that QInferGraph (Algorithm 4) identifies the latent graph correctly. But, F means that the algorithm fails to identify the latent graph. The results confirm our observations that we made in Model 1 (Part I). However, in this case QInferGraph has a higher performance quality. For example, for $\alpha=0.7,0.8,0.9,1$ we have: true positive rate (recall) = 1, false positive rate (fall-out) = 0, false negative rate (miss rate) = 0, accuracy = 1.

Table 6: Validation of Latent Graph in Model 2 (Part I) for $\alpha = 0.7, 0.8, 0.9, 1$, and $\beta \in (0.7, 0.8)$ via QInferGraph, and with the density matrix obtained from $0.6 \rho_{ZXY}^{1/\sqrt{2},1/\sqrt{2}} + 0.4 \rho_{ZXY}^{0.6,0.8}$ via tracing out Z.

						p_2	2					
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
	0.01	T	T	T	T	T	T	T	T	T	T	\mathbf{T}
	0.1	\mathbf{T}	${f T}$	${f T}$	${f T}$	${f T}$	${ m T}$	${ m T}$	${ m T}$	${ m T}$	${ m T}$	\mathbf{T}
	0.2	${f T}$	\mathbf{T}									
	0.3	\mathbf{T}										
	0.4	\mathbf{T}										
p_1	0.5	\mathbf{T}										
	0.6	\mathbf{T}	${f T}$	${f T}$	${f T}$	${f T}$	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}
	0.7	\mathbf{T}	${f T}$	${f T}$	${f T}$	${f T}$	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}
	0.8	\mathbf{T}	${f T}$	${f T}$	${f T}$	${f T}$	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}
	0.9	\mathbf{T}	${f T}$	${f T}$	${f T}$	${f T}$	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}
	0.99	T	\mathbf{T}	T								

Part II: Direct Graph. Assume that there are real numbers γ_1 , γ_2 , λ_1 , and λ_2 such that $\gamma_1^2 + \lambda_1^2 = 1$ and $\gamma_2^2 + \lambda_2^2 = 1$. We consider a joint entangled system (of two qubits) as the mixture of the following pure density matrices:

$$\begin{cases} \gamma_1^2|00\rangle + \gamma_1\lambda_1|01\rangle + \gamma_1\lambda_1|10\rangle + \lambda_1^2|11\rangle & q \\ \gamma_2^2|00\rangle + \gamma_2\lambda_2|01\rangle + \gamma_2\lambda_2|10\rangle + \lambda_2^2|11\rangle & 1-q \end{cases}$$

The system is a mixture of two pure density matrices. This quantum system has entanglement among the two quantum bits. Let the second quantum bit is transmitted over a quantum depolarizing channel with error probability p. With this setup, the joint density matrix is given as $\rho_{XY} = q\rho_{XY}^{\gamma_1,\lambda_1} + (1-q)\rho_{XY}^{\gamma_2,\lambda_2}$, where $\rho_{XY}^{\gamma,\lambda}$ is given as the mixture of the following pure density matrices:

$$\begin{cases} \gamma^2|00\rangle + \gamma\lambda|01\rangle + \gamma\lambda|10\rangle + \lambda^2|11\rangle & 1-p\\ \gamma^2|00\rangle - \gamma\lambda|01\rangle + \gamma\lambda|10\rangle - \lambda^2|11\rangle & p/3\\ \gamma\lambda|00\rangle + \gamma^2|01\rangle + \lambda^2|10\rangle + \gamma\lambda|11\rangle & p/3\\ -\gamma\lambda|00\rangle + \gamma^2|01\rangle - \lambda^2|10\rangle + \gamma\lambda|11\rangle & p/3 \end{cases}$$

We note that X and Y coexist in the quantum system, and thus the joint density matrix has been obtained. We already know that X is the cause of Y in this scenario, i.e., $X \to Y$ is the corresponding directed graph. To verify this, we use Algorithm 3 and 4 as we explained earlier in this model. The results are summarized in Table 7. T means that QInferGraph (Algorithm 4) identifies the direct graph correctly. But, F means that the algorithm fails to identify the direct graph. In all cases the probability of X be in state X_1 is q=0.4. Results show that the best performance belongs to $\alpha=0.9$ with only one false positive case. In general, in quantum noisy channels with very small probability of errors, QInferGraph very likely fails to draw the right conclusion about the identification of latent confounders.

Table 7: Validation of Direct Graph in Model 2 (Part II) with joint density matrix $\rho_{XY} = 0.4 * \rho_{XY}^{0.6,0.8} + 0.6 * \rho_{XY}^{1/\sqrt{2},1/\sqrt{2}}$.

						p						
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
	0.7	\mathbf{F}	F	T	T	T	T	T	T	T	T	\mathbf{T}
	0.8	\mathbf{F}	\mathbf{F}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	$\frac{\mathbf{T}}{\mathbf{T}}$
α	0.9	\mathbf{F}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	T
	1	F	\mathbf{F}	$\overset{-}{\mathrm{T}}$	\mathbf{T}							

5. Why Should We Not Map Quantum to Classical Directly?

Here, we show why classical common entropy approach do not directly apply to the quantum case. We emphasize that although a joint density operator (matrix) can be converted to a joint probability distribution (as explained in Example 1), we lose some quantum information due to the loss of entanglement. We give an example that shows converting a joint density matrix ρ_{XY} directly to a joint probability distribution p(X,Y), and then applying classical common entropy approach on p(X,Y) will not lead to the correct results.

Algorithm 5: Rotational procedure for computing the joint probability distribution of a joint density matrix

```
Input: Joint density matrix of quantum systems X and Y i.e., \rho_{XY}.

Output: Joint probability distribution p(X,Y) corresponding to the joint density matrix \rho_{XY}.

/* Compute eigenvalues and eigenvectors of \rho_X.

1 [V_1,D_1]=eig(\rho_X);

/* Compute eigenvalues and eigenvectors of \rho_Y.

2 [V_2,D_2]=eig(\rho_Y);

/* Rotational procedure

*/

3 U=V_1\otimes V_2;

4 \rho'_{XY}=U^\dagger\rho_{XY}U;

5 return p(X,Y) as the entries on the main diagonal of \rho'_{XY}.
```

Example 1 (Counter Example) Assume the depolarizing channel as described in Model 2, Part II. We already know that X causes Y in this model. To convert the joint density matrix ρ_{XY} , we use a rotational procedure explained as follows: Assume that ρ_{XY} is rotated

using a unitary matrix U. Let us say $\rho_{XY} = U \rho'_{XY} U^{\dagger}$. So, the joint density matrix ρ'_{XY} is computed as $\rho'_{XY} = U^{\dagger} \rho_{XY} U$. To compute the unitary matrix U for a given ρ_{XY} we use the eigenspaces of ρ_X and ρ_Y , where $\rho_X = \mathbf{Tr}_Y(\rho_{XY})$ and $\rho_Y = \mathbf{Tr}_X(\rho_{XY})$ are computed by tracing out Y and X, respectively. This simple observation enables us to design a procedure that converts a joint density matrix ρ_{XY} to a joint probability distribution p(X,Y) in a way that it takes into account the rotation. This procedure is formally described in Algorithm 5. By converting the joint density matrix ρ_{XY} directly to a joint probability distribution p(X,Y), using Algorithm 5, and then applying classical entropic causal inference, i.e., Algorithm 2 on p(X,Y) we obtain the results represented in Table 8 which are opposite to the expected results in all cases. This confirms that classical statistics are not adequate for identification of cause-effect relations in quantum systems due to accessibility of a richer spectrum of causal relations in quantum scenarios.

Table 8: Classical Approach to Identify Direct Graph for Model 2 does not work.

						p						
		0.01										0.99
	0.7	F	F	F	F	F	F	F	F	F	F	F
	0.8	\mathbf{F}	F F									
α	0.9	\mathbf{F}	F'	F'								
	1	F	\mathbf{F}	F								

Conclusions and Future Work

This paper provides a new approach for quantum entropic causal inference in the presence of hidden common causes. As a part of the approach, an iterative algorithmic solution is provided for the optimization problem that deals with the trade-off between the entropy of the latent quantum system and the quantum conditional mutual information of the observed quantum systems. The approach is validated on quantum noisy link, where the approach detects the expected causal relation. The extension of the problem to general quantum causality graph relations between multiple variables is an open problem for the future.

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Appendix A. Evaluation on Quantum Causal Synthetic Data: Generalized Quantum Symmetric Channel (Model 3)

In this section, we apply QInferGraph to a generalized version of binary symmetric channel, as explained in Model 3, where a qubit is transmitted over a binary symmetric channel (to illustrate the case of no confounder), or a qubit is transmitted over two separate channels (to illustrate the case of latent confounder). To build the model, we follow the same scheme that we explained in Model 1.

Model 3 (Generalized Quantum Symmetric Channel: Latent and Direct Graph) Part I: Latent Graph. Assume that there are real numbers γ and λ such that $\gamma^2 + \lambda^2 = 1$, and $X_1 = Y_1 = Z_1 = \gamma |0\rangle + \lambda |1\rangle$, and $X_2 = Y_2 = Z_2 = \gamma |0\rangle - \lambda |1\rangle$. Let Z be in the mixed state $|Z_1\rangle|X_1\rangle|Y_1\rangle$ with probability q, and $|Z_2\rangle|X_2\rangle|Y_2\rangle$ with probability 1-q. We consider a generalization of Quantum Symmetric Channel in the following model, in which the phase of the qubit is reversed with certain probability. The second and third qubits are transmitted over two separate quantum symmetric channels with error probability p_1 and p_2 , respectively, and are labeled X and Y, respectively. Thus, the joint density matrix of X, Y and Z, $\rho_{ZXY}^{\gamma,\lambda}$, can be written as mixtures of the following pure density matrices:

```
 \begin{cases} |Z_1\rangle|X_1\rangle|Y_1\rangle(|Z_1\rangle|X_1\rangle|Y_1\rangle)^{\dagger} & q(1-p_1)(1-p_2) \\ |Z_1\rangle|X_1\rangle|Y_2\rangle(|Z_1\rangle|X_1\rangle|Y_2\rangle)^{\dagger} & q(1-p_1)p_2 \\ |Z_1\rangle|X_2\rangle|Y_1\rangle(|Z_1\rangle|X_2\rangle|Y_1\rangle)^{\dagger} & qp_1(1-p_2) \\ |Z_1\rangle|X_2\rangle|Y_2\rangle(|Z_1\rangle|X_2\rangle|Y_2\rangle)^{\dagger} & qp_1p_2 \\ |Z_2\rangle|X_1\rangle|Y_1\rangle(|Z_2\rangle|X_1\rangle|Y_1\rangle)^{\dagger} & (1-q)p_1p_2 \\ |Z_2\rangle|X_1\rangle|Y_2\rangle(|Z_2\rangle|X_1\rangle|Y_2\rangle)^{\dagger} & (1-q)p_1(1-p_2) \\ |Z_2\rangle|X_2\rangle|Y_1\rangle(|Z_2\rangle|X_2\rangle|Y_1\rangle)^{\dagger} & (1-q)(1-p_1)p_2 \\ |Z_2\rangle|X_2\rangle|Y_2\rangle(|Z_2\rangle|X_2\rangle|Y_2\rangle)^{\dagger} & (1-q)(1-p_1)p_2 \end{cases}
```

Now, we trace out Z to obtain the density matrix for the latent graph $X \leftrightarrow Y$. Then, we apply QInferGraph (Algorithm 4) on ρ_{XY} to verify that X and Y are confounded by Z. For this purpose, we use QLatentSearch (Algorithm 3) on 50 different values of β , uniformly spaced in the interval (0.7,0.8). More results for $\beta \in (0.2,0.3)$, $\beta \in (0.6,0.7)$, and $\beta \in (0.8,0.9)$ can be found at the end of this section. We run QLatentSearch for 500 iterations each time. We use the conditional mutual information threshold of 0.05. In other words, of the algorithm outputs for the 50 β values used, we pick the smallest entropy W discovered by the algorithm among those that ensure $I(X;Y|W) \leq 0.05$. Table 9 summarizes the results for different S(W) threshold that is determined by $\theta = \alpha \min\{S(X), S(Y)\}$. For different values of $\alpha = 0.7, 0.8, 0.9, 1$, the results are the same, and are given in Table 9. We let q = 0.4. In the Table, T means that QInferGraph (Algorithm 4) identifies the latent graph correctly. But, F means that the algorithm fails to identify the latent graph. For very small or very large p_i 's the case of latent confounder or direct graph are hard to separate, while the proposed algorithm works well in most other cases.

Some highlights for results in Part I: (1) Note that where the probability of errors i.e., p_1 and p_2 are very small, the latent confounder Z is hardly distinguishable from X (or Y) and QInferGraph fails to discover the latent graph. (2) Note that QLatentSearch tries to find the stationary point(s) of the loss function L in Equation (2), and there is no quarantee to find the global optimum. However, the performance of QInferGraph in this

Table 9:	Validation of Latent	Graph in	Model 3 (F	Part I) i	for α	= 0.7, 0.8, 0.9, 1	with the
density r	matrix obtained from	$ ho_{ZXY}^{1/\sqrt{2},1/\sqrt{2}}$	via tracing	out Z .			

						p_2	2					
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
	0.01	F	F	F	T	T	T	T	T	F	F	F
	0.1	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	${ m T}$	\mathbf{F}	\mathbf{F}	\mathbf{F}
	0.2	\mathbf{F}	\mathbf{T}	\mathbf{F}								
	0.3	${f T}$	\mathbf{T}									
	0.4	${f T}$	\mathbf{T}									
p_1	0.5	${ m T}$	\mathbf{T}									
	0.6	${f T}$	\mathbf{T}									
	0.7	${f T}$	\mathbf{T}	\mathbf{T}	\mathbf{T}	${ m T}$	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}
	0.8	\mathbf{F}	${f T}$	${f T}$	${f T}$	${f T}$	\mathbf{T}	${ m T}$	\mathbf{T}	\mathbf{T}	${f T}$	\mathbf{F}
	0.9	\mathbf{F}	\mathbf{F}	\mathbf{F}	${f T}$	${f T}$	\mathbf{T}	${ m T}$	\mathbf{T}	\mathbf{F}	\mathbf{F}	\mathbf{F}
	0.99	F	\mathbf{F}	\mathbf{F}	${f T}$	${ m T}$	\mathbf{T}	\mathbf{T}	${ m T}$	\mathbf{F}	\mathbf{F}	F

case is acceptable: true positive rate (recall) = 0.77, false positive rate (fall-out) = 0, false negative rate (miss rate) = 0.23, accuracy = 0.77. (3) The hyperparameter α does not affect significantly on the quality of results in our experimental settings that indicates QInferGraph is not very sensitive to hyperparameters.

Part II: Direct Graph. We consider a generalization of Quantum Symmetric Channel in the following model, in which the phase of the qubit is reversed with certain probability. We consider a mixed state $|X_1\rangle|Y_1\rangle$ with probability q, and $|X_2\rangle|Y_2\rangle$ with probability 1-q. Further, the second qubit is transmitted over the quantum symmetric channel with the error probability p. After the transmission, the two qubits are labeled X and Y, respectively. Thus, the joint density matrix of X and Y is the mixture of the following pure density matrices:

$$\begin{cases} |X_1\rangle|Y_1\rangle(|X_1\rangle|Y_1\rangle)^{\dagger} & q(1-p) \\ |X_1\rangle|Y_2\rangle(|X_1\rangle|Y_2\rangle)^{\dagger} & qp \\ |X_2\rangle|Y_1\rangle(|X_2\rangle|Y_1\rangle)^{\dagger} & (1-q)p \\ |X_2\rangle|Y_2\rangle(|X_2\rangle|Y_2\rangle)^{\dagger} & (1-q)(1-p) \end{cases}$$

We already know that X is the cause of Y in this scenario, i.e., $X \to Y$ is the corresponding directed graph. To verify this, we use Algorithm 3 and 4 as we explained earlier in this model. The results are summarized in Table 10 for q=0.4. T means that QInferGraph (Algorithm 4) identifies the direct graph correctly. But, F means that the algorithm fails to identify the direct graph. In all cases for the different values of α considered, the results show that there is no false positive in this case indicating the desired causal inference.

Figure 5 illustrates the trade-off between the von Neumann entropy of the latent common cause and the conditional quantum mutual information of the observed systems for two examples of Model 3 in Part I and Part II. The conditional quantum mutual information between 0 and 0.05 in the I-S plot indicates that the suitable conditional quantum mutual information threshold for this setting is ≈ 0.05 .

Remark 1 Note that the generalized quantum symmetric channel is a rotated version of the classical binary symmetric channel. So, in this case we can convert the joint density

Table 10: Validation of Direct Graph in Model 3 (Part II) with the density matrix $\rho_{XY}^{1/\sqrt{2},1/\sqrt{2}}$.

						p)					
												0.99
	0.7	\mathbf{T}	T	T	T	T	T	T	T	T	T	T
	0.8	\mathbf{T}										
α	0.9	\mathbf{T}										
	1	\mathbf{T}	T T T									

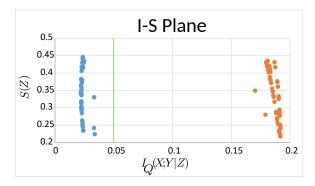


Figure 5: Trade-off curve discovered by QLatentSearch for: (i) Model 3 (Part I) with q=0.4 and p=0.1 [right-side curve], (ii) Model 3 (Part II) with q=0.4, $p_1=0.2$, and $p_2=0.3$ [left-side curve].

matrix to a joint probability distribution using the rotational procedure in Algorithm 5, we discuss this procedure later in Example 1. Then, we can apply the classical causal inference algorithm i.e., Algorithm 2 to identify latent confounders. However, our results in Table 11 and 12 indicate that even in this classical scenario our quantum approach outperforms the classical causal inference method. Note that there always exist a trade off for choosing $\alpha = 0.7, 0.8, 0.9, 1$ (and hence the H(Z) threshold). As suggested and verified in (Kocaoglu et al., 2020), $\alpha = 0.8$ seems an appropriate value for α in practice. Our results verifies this suggestion as well.

Table 11: Validation of Latent Graph in Model 3 (Part I) via classical causal inference (Algorithm 2).

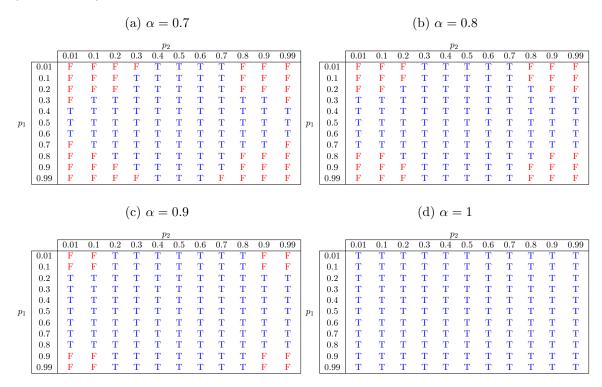


Table 12: Validation of Direct Graph in Model 3 (Part II) via classical causal inference (Algorithm 2).

						p						
		0.01		0.2								0.99
	0.7	T	T	T	T	F	F	F	T	T	T	\mathbf{T}
	0.8	\mathbf{T}	\mathbf{T}	${ m T}$	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{T}	\mathbf{T}	\mathbf{T}
α	0.9	\mathbf{T}	\mathbf{T}	T F	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{F}	\mathbf{T}	\mathbf{T}	\mathbf{T}
	1	\mathbf{F}										

To find the best choice of hyper-parameters in QInferGraph i.e., α and β , we evaluate the performance of QInferGraph for causal structure discovery in Model 3 by considering different intervals for the value of β and different values of α . Then, we will discuss the best choice of α and β in these settings.

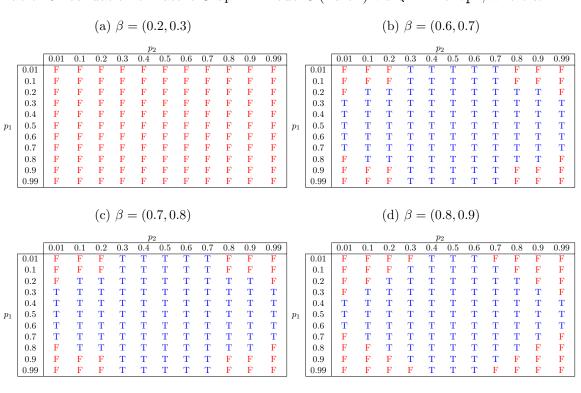
Part I: Latent Graph. In this part, we evaluate the performance of QInferGraph for the identification of latent graphs in Model 3 (Part I) as follows. We run QLatentSearch (Algorithm 1) on 50 different values of β uniformly spaced in the intervals (0.2,0.3), (0.6,0.7), (0.7,0.8), and (0.8,0.9), respectively. QInferGraph (Algorithm 2) calls QLatentSearch, and for each β the algorithm QLatentSearch is executed for 500 iterations. For different values of $\alpha = 0.7, 0.8, 0.9, 1$ the results are summarized in the following tables (Table 13, 14, 15, and 16), respectively. In the tables, T means that QInferGraph (Algorithm 2) identifies the latent graph correctly. But, F means that the algorithm fails to identify the latent graph. For very small or very large p_i 's (probability of errors, see Model 3 for details) the case of latent confounder or direct graph are hard to separate, while the proposed algorithm i.e., QInferGraph works well in most other cases where β is in (0.6,0.7), (0.7,0.8), and (0.8,0.9).

Table 13: Validation of Latent Graph in Model 3 (Part I) via QInferGraph, where $\alpha = 0.7, 0.8$.

(a) $\beta = (0.2, 0.3)$									(b) $\beta = (0.6, 0.7)$																
						p_2													p_2						
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99			0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
	0.01	F	F	F	\mathbf{F}	F	F	F	F	F	F	F		0.01	F	F	F	T	T	T	\mathbf{T}	T	F	F	F
	0.1	F	F	F	F	F	F	F	F	F	F	F		0.1	F	F	F	T	\mathbf{T}	T	T	T	F	F	F
	0.2	F	F	F	\mathbf{F}	F	F	F	F	\mathbf{F}	F	F		0.2	F	\mathbf{T}	\mathbf{T}	T	T	T	T	T	T	T	F
	0.3	F	F	F	F	F	F	F	F	F	F	F	p_1	0.3	T	T	T	T	T	T	T	T	T	T	T
	0.4	F	F	F	F	F	F	F	F	F	F	F		0.4	T	\mathbf{T}	\mathbf{T}	T	\mathbf{T}	T	T	T	T	\mathbf{T}	T
p_1	0.5	F	F	F	\mathbf{F}	F	F	F	F	F	F	F		0.5	T	\mathbf{T}	\mathbf{T}	T	T	T	T	T	T	\mathbf{T}	T
	0.6	F	F	F	\mathbf{F}	F	F	F	F	\mathbf{F}	\mathbf{F}	F		0.6	T	T	T	T	\mathbf{T}	T	\mathbf{T}	T	T	T	T
	0.7	F	F	F	\mathbf{F}	F	F	F	F	F	\mathbf{F}	F		0.7	T	T	T	T	T	T	\mathbf{T}	T	T	T	T
	0.8	F	F	F	F	F	F	F	F	F	\mathbf{F}	F		0.8	F	T	T	T	T	T	\mathbf{T}	T	\mathbf{T}	\mathbf{T}	F
	0.9	F	F	F	\mathbf{F}	F	F	F	F	F	F	F		0.9	F	F	F	T	\mathbf{T}	T	T	T	\mathbf{F}	F	F
	0.99	F	F	F	F	F	F	F	F	F	F	F		0.99	F	F	F	Т	T	T	T	T	F	F	F
				(c)	β =	= (0.	7, 0	.8)									(d)	β =	= (0	.8,0	.9)				
				(c)	β =	= (0.	.7,0	.8)									(d)	β =	= (0	.8,0	.9)				
		0.01	0.1	. ,		p_2	2	,	0.7	0.0	0.0	0.00			0.01	0.1	,		p_2	2		0.7	0.0	0.0	0.00
	0.01	0.01	0.1	0.2	0.3	$p_2 = 0.4$	0.5	0.6	0.7	0.8	0.9	0.99		0.01	0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
	0.01	F	F	0.2 F	0.3 T	p_2 0.4 T	0.5 T	0.6 T	Т	F	F	F		0.01	F	F	0.2 F	0.3 F	0.4 T	0.5 T	0.6 T	F	F	F	F
	0.1	F F	F F	0.2 F F	0.3 T T	7 0.4 T T	0.5 T T	0.6 T T	T T	F F	F F	F F		0.1	F F	F F	0.2 F F	0.3 F T	7 0.4 T T	0.5 T T	0.6 T T	F T	F F	F F	F F
	0.1 0.2	F F F	F F T	0.2 F F T	0.3 T T T	p_2 0.4 T T T	0.5 T T T	0.6 T T T	T T T	F F T	F F T	F F F		0.1 0.2	F F F	F F F	0.2 F F T	0.3 F T T	7 0.4 T T T	0.5 T T T	0.6 T T T	F T T	F F T	F F F	F F F
	0.1 0.2 0.3	F F F	F F T	0.2 F F T	0.3 T T T	p_2 0.4 T T T T	0.5 T T T T	0.6 T T T	T T T	F F T	F F T	F F T		0.1 0.2 0.3	F F F	F F F	0.2 F F T	0.3 F T T	7 T T T T	0.5 T T T T	0.6 T T T T	F T T	F F T	F F T	F F F
n_{\star}	0.1 0.2 0.3 0.4	F F T T	F F T T	0.2 F F T T	0.3 T T T T	p_2 0.4 T T T T T	0.5 T T T T	0.6 T T T T	T T T T	F F T T	F F T T	F F F T	74	0.1 0.2 0.3 0.4	F F F T	F F F T	0.2 F F T T	0.3 F T T T	7 T T T T	0.5 T T T T	0.6 T T T T	F T T T	F F T T	F F F T	F F F T
p_1	0.1 0.2 0.3 0.4 0.5	F F T T	F F T T	0.2 F F T T T	0.3 T T T T T	p_{2} 0.4 T T T T T T	0.5 T T T T T	0.6 T T T T T	T T T T T	F F T T	F F T T	F F T T	p_1	0.1 0.2 0.3 0.4 0.5	F F F T	F F T T	0.2 F F T T T	0.3 F T T T	7 T T T T T T	0.5 T T T T T	0.6 T T T T T	F T T T T	F F T T	F F T T	F F F T
p_1	0.1 0.2 0.3 0.4 0.5 0.6	F F T T	F F T T T	0.2 F F T T T	0.3 T T T T T T	p_{2} 0.4 T T T T T T T	T T T T T T T	0.6 T T T T T T	T T T T T	F F T T T	F F T T T	F F T T T	p_1	0.1 0.2 0.3 0.4 0.5 0.6	F F F T T	F F T T T	0.2 F F T T T	0.3 F T T T T	7 T T T T T T T T	0.5 T T T T T T	0.6 T T T T T T	F T T T T	F F T T T	F F T T T	F F F T T
p_1	0.1 0.2 0.3 0.4 0.5 0.6 0.7	F F T T T	F F T T T T	0.2 F F T T T T	0.3 T T T T T T T	p_2 0.4 T T T T T T T T	0.5 T T T T T T	0.6 T T T T T T	T T T T T T	F T T T T T	F T T T T T	F F T T T	p_1	0.1 0.2 0.3 0.4 0.5 0.6 0.7	F F F T T	F F T T T	0.2 F F T T T T	0.3 F T T T T T	7 T T T T T T T T T T T T T T T T T T T	0.5 T T T T T T	0.6 T T T T T T	F T T T T T T	F F T T T T	F F T T T T	F F F T T
p_1	0.1 0.2 0.3 0.4 0.5 0.6 0.7	F F T T T T	F T T T T T	0.2 F F T T T T T	0.3 T T T T T T T	p_2 0.4 T	0.5 T T T T T T T	0.6 T T T T T T T T T T	T T T T T T T	F F T T T T T	F F T T T T T	F F T T T T	p_1	0.1 0.2 0.3 0.4 0.5 0.6 0.7	F F F T T F	F F T T T T	0.2 F F T T T T T	0.3 F T T T T T T	7 T T T T T T T T T T T T T T T T T T T	0.5 T T T T T T T	0.6 T T T T T T T	F T T T T T T	F F T T T T T	F F T T T T	F F F T T F
p_1	0.1 0.2 0.3 0.4 0.5 0.6 0.7	F F T T T	F F T T T T	0.2 F F T T T T	0.3 T T T T T T T	p_2 0.4 T T T T T T T T	0.5 T T T T T T	0.6 T T T T T T	T T T T T T	F T T T T T	F T T T T T	F F T T T	p_1	0.1 0.2 0.3 0.4 0.5 0.6 0.7	F F F T T	F F T T T	0.2 F F T T T T	0.3 F T T T T T	7 T T T T T T T T T T T T T T T T T T T	0.5 T T T T T T	0.6 T T T T T T	F T T T T T T	F F T T T T	F F T T T T	F F F T T

Table 14: Validation of Latent Graph in Model 3 (Part I) via QInferGraph, where $\alpha = 0.9$.

Table 15: Validation of Latent Graph in Model 3 (Part I) via QInferGraph, where $\alpha = 1$.



Part II: Direct Graph In this part we consider direct graphs in Model 3 (Part II), and we use the same parameters explained in Part I of this section. In all cases for the different values of α considered, the results show that there is no false positive in this case indicating the desired causal inference.

Table 16: Validation of Direct Graph in Model 3 (Part II) for β uniformly spaced in the intervals (0.2,0.3), (0.6,0.7), (0.7,0.8), and (0.8,0.9).

						p						
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
	0.7	\mathbf{T}	T	T	T	T	T	T	T	T	T	\mathbf{T}
	0.8	\mathbf{T}										
α	0.9	\mathbf{T}	$egin{array}{c} T \ T \end{array}$									
	1	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	${ m T}$	${ m T}$	${ m T}$	${ m T}$	\mathbf{T}

Appendix B. Evaluation on Quantum Causal Synthetic Data: Depolarizing Quantum Channel (Model 2)

To find the best choice of hyper-parameters in QInferGraph i.e., α and β , we evaluate the performance of QInferGraph for causal structure discovery in Model 2 by considering different intervals for the value of β and different values of α . Then, we will discuss the best choice of α and β in these settings.

Part I: Latent Graph. In this part, we evaluate the performance of QInferGraph for the identification of latent graphs in Model 2 (Part I) as follows. We run QLatentSearch (Algorithm 1) on 50 different values of β uniformly spaced in the interval (0.2,0.3), (0.6,0.7), (0.7,0.8), and (0.8,0.9), respectively. QInferGraph (Algorithm 2) calls QLatentSearch, and for each β the algorithm QLatentSearch is executed for 500 iterations. For different values of $\alpha = 0.7, 0.8, 0.9, 1$ the results are summarized in Table 17. In the table, T means that QInferGraph (Algorithm 2) identifies the latent graph correctly. But, F means that the algorithm fails to identify the latent graph. Our proposed algorithm i.e., QInferGraph works well where β is in (0.2,0.3), (0.6,0.7), (0.7,0.8), and (0.8,0.9). The results confirm our observations that we made in Model 3 (Part I). However, in this case QInferGraph has a higher performance quality, in almost all cases.

Table 17: Validation of Latent Graph in Model 2 (Part I) via QInferGraph, where $\alpha = 0.7, 0.8, 0.9, 1$ and $\beta \in (0.2, 0.3), (0.6, 0.7), (0.7, 0.8), (0.8, 0.9).$

						p_2	2					
		0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.99
	0.01	${ m T}$	T	T	T	T	T	T	T	T	T	\mathbf{T}
	0.1	${f T}$	${ m T}$	${f T}$	${f T}$	${f T}$	${ m T}$	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}
	0.2	${f T}$	\mathbf{T}									
	0.3	${f T}$	\mathbf{T}									
	0.4	${f T}$	\mathbf{T}									
p_1	0.5	${f T}$	\mathbf{T}									
	0.6	${f T}$	\mathbf{T}									
	0.7	${f T}$	\mathbf{T}	${f T}$	${f T}$	${f T}$	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}
	0.8	${f T}$	\mathbf{T}	${f T}$	${f T}$	${f T}$	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}
	0.9	${f T}$	${f T}$	${f T}$	${f T}$	${f T}$	${f T}$	\mathbf{T}	${f T}$	\mathbf{T}	${f T}$	\mathbf{T}
	0.99	${f T}$	${f T}$	${f T}$	${f T}$	${f T}$	${f T}$	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}	\mathbf{T}

Part II: Direct Graph In this part we consider direct graphs in Model 2 (Part II), and we use the same parameters explained in Part I of this section. In all cases for the different values of α considered, the results show that there is no false positive in this case indicating the desired causal inference. The results, Table 18, indicates that in quantum noisy channels with very small probability of errors, QInferGraph very likely fails to draw the right conclusion about the identification of latent confounders.

Table 18: Validation of Direct Graph in Model 2 (Part II).

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