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# Supplementary information

## Quantum theory cannot violate a causal inequality

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### I. EQUIVALENCE OF COMBINED AND INDIVIDUAL CONTROLLED LAB GATES

In this section we show that the framework for quantum processes in the main text is equivalent to considering any quantum circuit built up of standard unitary gates and controlled gates for individual laboratories, in terms of the probability distributions they can generate. The key ingredient is to show how to construct individual controlled lab gates from  $V$ , and conversely how to construct the operation  $V$  from individual controlled lab gates.

To map any circuit involving individual controlled lab gates into our framework, we first space out the gates in the circuit, so that there is only one gate per time-step (this will increase the depth, but not affect the results). If an individual lab gate acts on only part of the system, we extend it such that it acts on the entire system, taking the action to be trivial (i.e. tensored with the identity) on any part of the system which was not initially included. We can then replace each individual controlled lab gate by a circuit fragment involving one use of  $V$ , using the approach described below. Finally we merge all unitary gates between instances of  $V$  into the unitaries  $U_t$ . This will lead to a circuit in our framework yielding exactly the same results as the original circuit. To go in the other direction, we simply replace each instance of  $V$  with its construction in terms of individual controlled lab gates.

Figures 1 and 2 show how to construct an individual controlled lab gate using  $V$ . Figure 3 shows how to construct  $V$  from individual controlled lab gates.

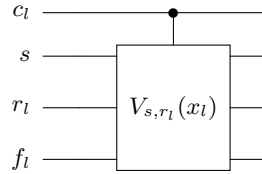


FIG. 1. A controlled lab gate for an individual laboratory

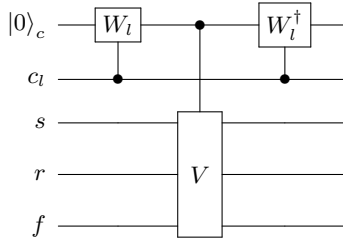


FIG. 2. An equivalent circuit to the individual controlled lab gate above, built from a single instance of  $V$ , where  $W_l |0\rangle = |l\rangle$ . Note that the individual wires may represent composite subsystems rather than individual qubits.

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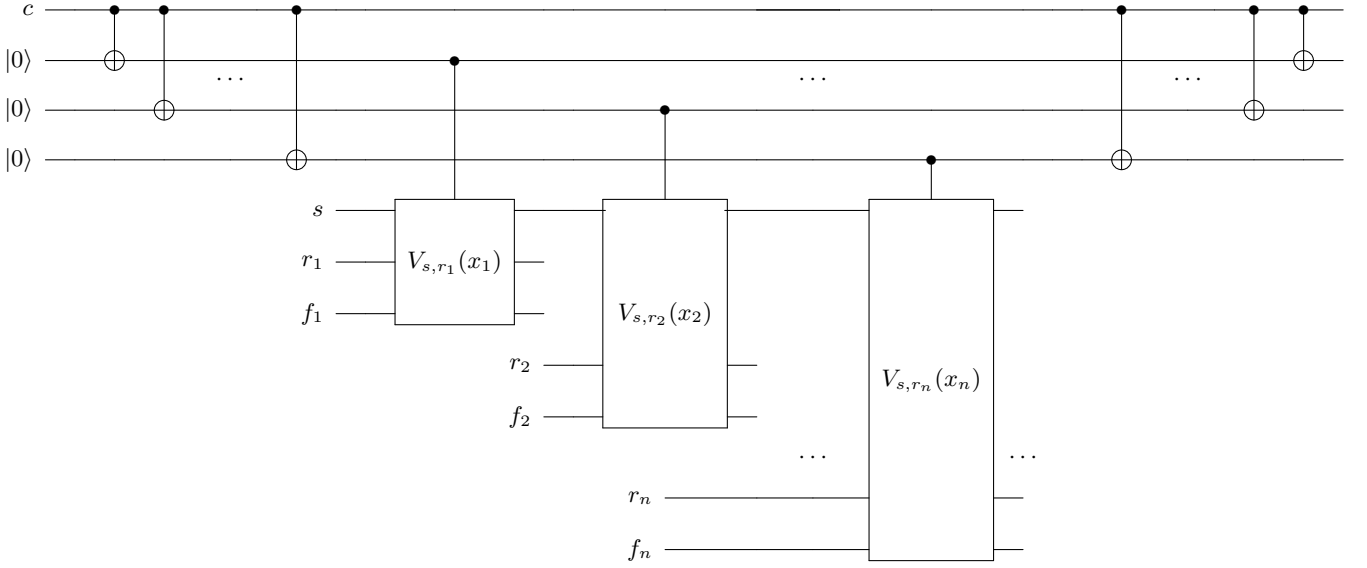


FIG. 3.  $V$ , built from individual controlled lab gates. The first and last  $CNOT$  gate are controlled from the state  $|1\rangle_c$ , the second and second from last are controlled from  $|2\rangle_c$ , and so on until the  $n$ 'th and  $n+1$ 'th  $CNOT$ , which are controlled from state  $|n\rangle_c$ .

## II. PROOF OF THE MAIN RESULT

In this supplementary information section, we give the full proof of the main result, that the probabilities generated by a quantum protocol can be replicated by a classical causal model, and therefore cannot violate a causal inequality. We begin with recalling a few definitions from the main text, together with some convenient derived quantities. Note that we assume throughout that laboratory labels  $l$  are non-zero.

**Definition 1** *A causal probabilistic model can be written as*

$$p(\vec{a}|\vec{x}) = \sum_{l_1 \notin \mathcal{L}_0} \sum_{l_2 \notin \mathcal{L}_1} \dots \sum_{l_N \notin \mathcal{L}_{N-1}} p_1(l_1|H_0) p_1(a_{l_1}|H_0, x_{l_1}) p_2(l_2|H_1) p_2(a_{l_2}|H_1, x_{l_2}) \dots p_N(l_N|H_{N-1}) p_N(a_{l_N}|H_{N-1}, x_{l_N}) \quad (1)$$

where  $p_k(l_k|H_{k-1})$  terms represent probabilities for party  $l_k$  to act at stage  $k$  of the causal order, and  $p_k(a_{l_k}|H_{k-1}, x_{l_k})$  terms represent probabilities for party  $l_k$ , who has acted at stage  $k$  of the causal order to obtain measurement result  $a_{l_k}$ . Both of the above probabilities are conditional on a history,  $H_{k-1}$ , which contains all of the information about previous inputs, outputs and party order. In particular, the history  $H_k = (h_1, \dots, h_k)$  is the ordered collection of triples  $h_k = (l_k, a_{l_k}, x_{l_k})$ . The summations are performed over all possible next parties, excluding parties who have already acted, which are stored in the unordered sets  $\mathcal{L}_k = \{l_1, \dots, l_k\}$ . To emphasise the symmetry between the terms we include  $H_0$  and  $\mathcal{L}_0$ , which are defined as empty sets, as no parties have acted at that point.

**Definition 2** *The state of the system with a History  $H_{k-1}$ , at a time given by  $t$ , with the control set to trigger the action of party  $l_k$  is given by*

$$|\psi_{(l_k, t, H_{k-1})}\rangle = (|l_k\rangle \langle l_k|_c \otimes \pi_{r_f}^{H_{k-1}} \otimes I) U_t V U_{t-1} \dots V U_1 |0\rangle. \quad (2)$$

The projector onto the result and flag spaces is given by  $\pi_{r_f}^{H_{k-1}} = \bigotimes_{i=1}^N \left( \pi_{r_i f_i}^{H_{k-1}} \right)$ , where

$$\pi_{r_i f_i}^{H_{k-1}} = \begin{cases} |a_i\rangle \langle a_i|_{r_i} \otimes |1\rangle \langle 1|_{f_i} & \text{if } (i, a_i, x_i) \in H_{k-1}, \\ I_{r_i} \otimes |0\rangle \langle 0|_{f_i} & \text{otherwise.} \end{cases} \quad (3)$$

We also define the same state evolved to the end of protocol to be

$$|\bar{\psi}_{(l_k, t, H_{k-1})}\rangle = V U_T V U_{T-1} \dots U_{t+1} V |\psi_{(l_k, t, H_{k-1})}\rangle. \quad (4)$$

It will also be convenient for the proof to define  $|\psi_{(0, t, H_{k-1})}\rangle$  and  $|\bar{\psi}_{(0, t, H_{k-1})}\rangle$ , which are the same as the above states, but with  $l_k = 0$  (i.e. the control in the 'do nothing' setting).

**Definition 3** The state of the system with a History  $H_k$ , at a time given by  $t$ , in which party  $l_k$  has just acted is given by

$$|\phi_{(l_k,t,H_k)}\rangle = (|a_{l_k}\rangle \langle a_{l_k}|_{\mathcal{R}_k} \otimes I)V|\psi_{(l_k,t,H_{k-1})}\rangle. \quad (5)$$

We also define the same state evolved to the end of protocol to be

$$|\bar{\phi}_{(l_k,t,H_k)}\rangle = VU_T VU_{T-1} \dots U_{t+1} |\phi_{(l_k,t,H_k)}\rangle. \quad (6)$$

It will also be convenient for the proof to define  $|\phi_{(0,t,H_k)}\rangle = V|\psi_{(0,t,H_k)}\rangle$  and  $|\bar{\phi}_{(0,t,H_k)}\rangle = VU_T VU_{T-1} \dots U_{t+1} |\phi_{(0,t,H_k)}\rangle$ .

**Definition 4** The probability for party  $l_k$  to act next, given a history  $H_{k-1}$  is given by:

$$p_k(l_k|H_{k-1}) = \frac{\sum_{t_k=1}^T ||\psi_{(l_k,t_k,H_{k-1})}\rangle|^2}{\sum_{l'_k \notin \mathcal{L}_{k-1}} \sum_{t'_k=1}^T ||\psi_{(l'_k,t'_k,H_{k-1})}\rangle|^2} \quad (7)$$

**Definition 5** The probability for party  $l_k$  to obtain the measurement result  $a_{l_k}$ , given a history  $H_{k-1}$ , and an input variable  $x_{l_k}$  is given by:

$$p_k(a_{l_k}|H_{k-1}, x_{l_k}) = \frac{\sum_{t_k=1}^T ||\phi_{(l_k,t_k,H_k)}\rangle|^2}{\sum_{a'_{l_k} \in \mathcal{A}_{l_k}} \sum_{t'_k=1}^T ||\phi_{(l_k,t'_k,H_k)}\rangle|^2} \quad (8)$$

where  $H'_k = (H_{k-1}, (l_k, a'_{l_k}, x_{l_k}))$  (i.e.  $H_k$  with  $a_{l_k}$  replaced by  $a'_{l_k}$ ).

**Definition 6** The quantum protocol consists of preparing an initial state  $|0\rangle$ , then acting with an alternating sequence of unitaries  $U_t$  that act on the system and the control, and unitaries  $V$  that act on the system, results and flag spaces as specified by the control. The total unitary for the protocol is given by

$$\mathcal{U} = VU_T VU_{T-1} V \dots VU_N V \dots VU_1 \quad (9)$$

where we note that for an  $N$  party protocol,  $T \geq N$ . Finally, the results registers are measured in the computational basis, giving the outcome probability distribution

$$p^{\text{quantum}}(\vec{a}|\vec{x}) = |(\langle \vec{a} | \otimes I) \mathcal{U} |0\rangle|^2. \quad (10)$$

With these definitions in place, we first prove some useful orthogonality lemmas concerning the barred states.

**Lemma 1** We have that

$$\langle \bar{\psi}_{l',t',H} | \bar{\psi}_{l,t,H} \rangle = 0 \quad (11)$$

unless  $l = l'$  and  $t' = t$ .

Proof: consider first that  $t = t'$  and  $l \neq l'$ . Then we have that  $\langle \bar{\psi}_{l',t,H} | \bar{\psi}_{l,t,H} \rangle = \langle \psi_{l',t,H} | \psi_{l,t,H} \rangle = 0$ , since  $|\psi_{l',t,H}\rangle$  and  $|\psi_{l,t,H}\rangle$  are orthogonal on the control  $\mathcal{H}_c$ . Next, consider that  $t < t'$ . Then  $\langle \bar{\psi}_{l',t',H} | \bar{\psi}_{l,t,H} \rangle = \langle \psi_{l',t',H} | U_{t'} V \dots U_{t+1} V | \psi_{l,t,H} \rangle = 0$  since  $V | \psi_{l,t,H} \rangle$  contains a raised  $l$  flag that is not raised in  $\langle \psi_{l',t',H} |$ , and there is no operator connecting the two which can lower this flag. The case with  $t > t'$  follows from the  $t < t'$  case by noting that  $\langle \bar{\psi}_{l',t',H} | \bar{\psi}_{l,t,H} \rangle = \langle \bar{\psi}_{l,t,H} | \bar{\psi}_{l',t',H} \rangle^*$ .

**Lemma 2** We have that

$$\langle \bar{\phi}_{l',t',H} | \bar{\phi}_{l,t,H} \rangle = 0 \quad (12)$$

unless  $l = l'$  and  $t = t'$ .

Proof: consider first that  $t = t'$  and  $l \neq l'$ . Then we have that  $\langle \bar{\phi}_{l',t,H} | \bar{\phi}_{l,t,H} \rangle = \langle \phi_{l',t,H} | \phi_{l,t,H} \rangle = 0$ , since  $|\phi_{l',t,H}\rangle$  and  $|\phi_{l,t,H}\rangle$  are orthogonal on the control  $\mathcal{H}_c$ . Next, consider that  $t < t'$ . Then  $\langle \bar{\phi}_{l',t',H} | \bar{\phi}_{l,t,H} \rangle = \langle \phi_{l',t',H} | VU_{t'} V \dots U_{t+1} | \phi_{l,t,H} \rangle = 0$ , since the leftmost  $V$  either raises a flag not in the history  $H$ , or the control at this point is set to zero, either of which will give the desired orthogonality. The case with  $t > t'$  follows from the  $t < t'$  case by noting that  $\langle \bar{\phi}_{l',t',H} | \bar{\phi}_{l,t,H} \rangle = \langle \bar{\phi}_{l,t,H} | \bar{\phi}_{l',t',H} \rangle^*$ .

We now move onto proving the main result. This will consist of four stages, the first concerns a cancellation within terms of the same causal order stage, which allows us to rewrite the causal model in a nice way. The second and third results concern the initial and final terms in the inductive proof. The former corresponds to the fact that ‘somebody has to measure first’ in the quantum protocol, and the latter that the final term in the causal model has sufficient expressive power to capture the quantum measurement probabilities in their entirety. Finally, the fourth result concerns cancellations between terms at subsequent stages of the causal order. This leads to our main result which ties all of this together for a full proof that  $p(\vec{a}|\vec{x}) = |\langle 0|U|0\rangle|^2$  is causal.

**Result 1** *There is an equality between the numerator of the ‘who is next’ type probabilities  $p_k(l_k|H_{k-1})$ , and the denominator of the ‘results’ type probabilities  $p_k(a_{l_k}|H_{k-1}, x_{l_k})$ , allowing us to write the product of these probabilities in a nice way as*

$$p_k(l_k|H_{k-1})p_k(a_{l_k}|x_{l_k}, H_{k-1}) = \frac{\sum_{t_k=1}^T |\phi_{(l_k, t_k, H_k)}\rangle|^2}{\sum_{l'_k \notin \mathcal{L}_{k-1}} \sum_{t'_k=1}^T |\psi_{(l'_k, t'_k, H_{k-1})}\rangle|^2}. \quad (13)$$

Proof: Starting with the denominator of the ‘results’ probability

$$\begin{aligned} \sum_{a'_{l_k} \in \mathcal{A}_{l_k}} \sum_{t_k=1}^T |\phi_{(l_k, t_k, H'_k)}\rangle|^2 &= \sum_{a'_{l_k} \in \mathcal{A}_{l_k}} \sum_{t_k=1}^T \left| \langle a'_{l_k} \rangle \langle a'_{l_k} |_{r_k} \otimes \mathcal{I} V |\psi_{(l_k, t_k, H_{k-1})}\rangle \right|^2 \\ &= \sum_{t_k=1}^T \left| \sum_{a'_{l_k} \in \mathcal{A}_{l_k}} \langle a'_{l_k} \rangle \langle a'_{l_k} |_{r_k} \otimes \mathcal{I} V |\psi_{(l_k, t_k, H_{k-1})}\rangle \right|^2 \\ &= \sum_{t_k=1}^T |V |\psi_{(l_k, t_k, H_{k-1})}\rangle|^2 \end{aligned} \quad (14)$$

$$= \sum_{t_k=1}^T |\psi_{(l_k, t_k, H_{k-1})}\rangle|^2, \quad (15)$$

we obtain the numerator of the ‘who is next’ probabilities. In the second line we have used orthogonality on the results register, in the third line we have used the fact that after a measurement by party  $l_k$ , some result in  $\mathcal{A}_{l_k}$  must have been obtained, and in the final line we have used unitarity. Using this to cancel the numerator of (7) with the denominator of (8) we obtain the desired result.

**Result 2** *The denominator of the first term  $p_1(l_1|H_0)$  satisfies*

$$\sum_{l_1 \notin \mathcal{L}_0} \sum_{t_1=1}^T |\psi_{(l_1, t_1, H_0)}\rangle|^2 = 1. \quad (16)$$

Proof: by first using unitarity and then Lemma 1 we have

$$\begin{aligned} \sum_{l_1 \notin \mathcal{L}_0} \sum_{t_1=1}^T |\psi_{(l_1, t_1, H_0)}\rangle|^2 &= \sum_{l_1 \notin \mathcal{L}_0} \sum_{t_1=1}^T |\bar{\psi}_{(l_1, t_1, H_0)}\rangle|^2 \\ &= \left| \sum_{l_1 \notin \mathcal{L}_0} \sum_{t_1=1}^T \bar{\psi}_{(l_1, t_1, H_0)} \right|^2. \end{aligned} \quad (17)$$

To simplify this further, consider evolving the state  $|\psi_{0, t_1-1, H_0}\rangle$  forward for a full time-step using  $U_{t_1}V$ . As the control is in state 0, no measurement occurs during  $V$ , and the unitary  $U_1$  creates a superposition in which the control takes any possible state. Symbolically,

$$U_{t_1}V |\psi_{0, t_1-1, H_0}\rangle = \sum_{l_1 \notin \mathcal{L}_0} |\psi_{(l_1, t_1, H_0)}\rangle + |\psi_{(0, t_1, H_0)}\rangle. \quad (18)$$

By applying  $VU_T V \dots U_{t_1+1} V$  to this equation, we can obtain a similar form for the barred states,

$$|\bar{\psi}_{0,t_1-1,H_0}\rangle = \sum_{l_1 \notin \mathcal{L}_0} |\bar{\psi}_{(l_1,t_1,H_0)}\rangle + |\bar{\psi}_{(0,t_1,H_0)}\rangle. \quad (19)$$

We can rearrange this equation and substitute for the sum over  $l_1$  on the right-hand side of (17) to obtain

$$\sum_{l_1 \notin \mathcal{L}_0} \sum_{t_1=1}^T |\psi_{(l_1,t_1,H_0)}\rangle|^2 = \left| \sum_{t_1=1}^T (|\bar{\psi}_{(0,t_1-1,H_0)}\rangle) - |\bar{\psi}_{(0,t_1,H_0)}\rangle \right|^2 \quad (20)$$

By expanding the summation on the right-hand side we find that only the first and last terms remain, giving

$$\sum_{l_1 \notin \mathcal{L}_0} \sum_{t_1=1}^T |\psi_{(l_1,t_1,H_0)}\rangle|^2 = \left| |\bar{\psi}_{(0,0,H_0)}\rangle - |\bar{\psi}_{(0,T,H_0)}\rangle \right|^2 \quad (21)$$

Note that it is impossible by the requirements of our protocol that no-one has measured by time  $t = T$ . Such a scenario would violate the assumption that there are exactly  $N$  flags raised at the end of the protocol. Therefore,  $|\bar{\psi}_{(0,T,H_0)}\rangle = 0$ , and we find

$$\sum_{l_1 \notin \mathcal{L}_0} \sum_{t_1=1}^T |\psi_{(l_1,t_1,H_0)}\rangle|^2 = \left| |\bar{\psi}_{(0,0,H_0)}\rangle \right|^2 = |\mathcal{U}|0\rangle|^2 = 1 \quad (22)$$

as desired.

**Result 3** *The outcome statistics in the numerator of the final term in the causal probabilistic model represent the quantum probabilities arising from the protocol. In other words,*

$$\sum_{l_N \in \mathcal{L}_N} \sum_{t_N=1}^T |\phi_{(l_N,t_N,H_N)}\rangle|^2 = \left| \langle \vec{a} | \langle \vec{a} | \otimes I \mathcal{U} |0\rangle \right|^2 \quad (23)$$

Proof: Firstly, note that by unitarity and Lemma 2 we have that

$$\begin{aligned} \sum_{l_N \in \mathcal{L}_N} \sum_{t_N=1}^T |\phi_{(l_N,t_N,H_N)}\rangle|^2 &= \sum_{l_N \in \mathcal{L}_N} \sum_{t_N=1}^T |\bar{\phi}_{(l_N,t_N,H_N)}\rangle|^2 \\ &= \left| \sum_{l_N \in \mathcal{L}_N} \sum_{t_N=1}^T |\bar{\phi}_{(l_N,t_N,H_N)}\rangle \right|^2. \end{aligned} \quad (24)$$

The history  $H_N$  represents a case in which all parties have already measured. At time  $t < T$ , what are the possible ways that this history can be filled? Either, nobody has measured in the previous time-step, or the last party to be filled into the history (subject to the requirement every party must enter the history exactly once) has just measured. In any case, evolving the linear combination of these states forward a time-step must produce a state at  $t + 1$  which contains an empty control (i.e., no-one else is left to measure, so don't trigger them!). This gives us the key relation

$$VU_{t+1} \left( \sum_{l_N \in \mathcal{L}_N} |\phi_{(l_N,t,H_N)}\rangle + |\phi_{(0,t,H_N)}\rangle \right) = |\phi_{(0,t+1,H_N)}\rangle \quad (25)$$

which holds for  $t < T$ . Applying  $VU_T V \dots U_{t+2}$  we obtain

$$\left( \sum_{l_N \in \mathcal{L}_N} |\bar{\phi}_{(l_N,t,H_N)}\rangle + |\bar{\phi}_{(0,t,H_N)}\rangle \right) = |\bar{\phi}_{(0,t+1,H_N)}\rangle \quad (26)$$

which we can then rearrange to get

$$\sum_{l_N \in \mathcal{L}_N} |\bar{\phi}_{(l_N,t,H_N)}\rangle = |\bar{\phi}_{(0,t+1,H_N)}\rangle - |\bar{\phi}_{(0,t,H_N)}\rangle. \quad (27)$$

By separating out the  $t_N = T$  term in equation (24) and then substituting this in the remaining terms, we find that

$$\begin{aligned}
\sum_{l_N \in \mathcal{L}_N} \sum_{t_N=1}^T ||\phi_{(l_N, t_N, H_N)}\rangle|^2 &= \left| \sum_{l_N \in \mathcal{L}_N} |\bar{\phi}_{(l_N, T, H_N)}\rangle + \sum_{t_N=1}^{T-1} \sum_{l_N \in \mathcal{L}_N} |\bar{\phi}_{(l_N, t_N, H_N)}\rangle \right|^2 \\
&= \left| \sum_{l_N \in \mathcal{L}_N} |\bar{\phi}_{(l_N, T, H_N)}\rangle + \sum_{t_N=1}^{T-1} (|\bar{\phi}_{(0, t_N+1, H_N)}\rangle - |\bar{\phi}_{(0, t_N, H_N)}\rangle) \right|^2 \\
&= \left| \sum_{l_N \in \mathcal{L}_N} |\bar{\phi}_{(l_N, T, H_N)}\rangle + |\bar{\phi}_{(0, T, H_N)}\rangle - |\bar{\phi}_{(0, 1, H_N)}\rangle \right|^2.
\end{aligned} \tag{28}$$

Now we note that  $|\bar{\phi}_{(0, 1, H_N)}\rangle = 0$  since it would be impossible for all parties to have measured in one time-step, and for the control to be in the zero state. Then we note that  $\sum_{l_N \in \mathcal{L}_N} |\bar{\phi}_{(l_N, T, H_N)}\rangle + |\bar{\phi}_{(0, T, H_N)}\rangle = (\pi_{rf}^{H_N} \otimes I)\mathcal{U}|0\rangle$ , which is to say that these are simply the possible states at the end of the protocol, containing the measurement results we want to calculate the probabilities for in the history. Therefore

$$\begin{aligned}
\sum_{l_N \in \mathcal{L}_N} \sum_{t_N=1}^T ||\phi_{(l_N, t_N, H_N)}\rangle|^2 &= |(\pi_{rf}^{H_N} \otimes I)\mathcal{U}|0\rangle|^2 \\
&= |(|\vec{a}\rangle \langle \vec{a}| \otimes I)\mathcal{U}|0\rangle|^2
\end{aligned} \tag{29}$$

as desired.

**Result 4** *This is a technical result which establishes an equality between the states after measurement at causal order stage  $k$  and the states before measurement at the next stage of the causal order. Namely, for  $1 \leq k < N$  that:*

$$\sum_{l_k \in \mathcal{L}_k} \sum_{t=1}^T ||\phi_{(l_k, t, H_k)}\rangle|^2 = \sum_{t'=1}^T \sum_{l'_{k+1} \notin \mathcal{L}_k} ||\psi_{(l'_{k+1}, t', H_k)}\rangle|^2. \tag{30}$$

Proof: Firstly, by unitarity and Lemma 2 we have that

$$\begin{aligned}
\sum_{l_k \in \mathcal{L}_k} \sum_{t=1}^T ||\phi_{(l_k, t, H_k)}\rangle|^2 &= \sum_{l_k \in \mathcal{L}_k} \sum_{t=1}^T ||\bar{\phi}_{(l_k, t, H_k)}\rangle|^2 \\
&= \left| \sum_{l_k \in \mathcal{L}_k} \sum_{t=1}^T |\bar{\phi}_{(l_k, t, H_k)}\rangle \right|^2.
\end{aligned} \tag{31}$$

Consider time-evolving a state just after the  $t^{\text{th}}$  measurement step, in which history  $H_k$  has been obtained (either by the last party just having measured, or by all parties in  $H_k$  having measured previously), by  $U_{t+1}$ . This links states of the form  $|\phi_{(l_k, t, H_k)}\rangle$  and  $|\psi_{(l'_{k+1}, t+1, H_k)}\rangle$  via

$$U_{t+1} \left( \sum_{l_k \in \mathcal{L}_k} |\phi_{(l_k, t, H_k)}\rangle + |\phi_{(0, t, H_k)}\rangle \right) = \sum_{l'_{k+1} \notin \mathcal{L}_k} |\psi_{(l'_{k+1}, t+1, H_k)}\rangle + |\psi_{(0, t+1, H_k)}\rangle \tag{32}$$

for  $t < T$ . Applying  $VU_T V \dots U_{t+2} V$  we obtain a very similar result for barred states;

$$\sum_{l_k \in \mathcal{L}_k} |\bar{\phi}_{(l_k, t, H_k)}\rangle + |\bar{\phi}_{(0, t, H_k)}\rangle = \sum_{l'_{k+1} \notin \mathcal{L}_k} |\bar{\psi}_{(l'_{k+1}, t+1, H_k)}\rangle + |\bar{\psi}_{(0, t+1, H_k)}\rangle. \tag{33}$$

We also note that  $|\phi_{(0, t, H_k)}\rangle = V|\psi_{(0, t, H_k)}\rangle$  and hence that  $|\bar{\phi}_{(0, t, H_k)}\rangle = |\bar{\psi}_{(0, t, H_k)}\rangle$ . Making this substitution and rearranging a little we get

$$\sum_{l_k \in \mathcal{L}_k} |\bar{\phi}_{(l_k, t, H_k)}\rangle = \sum_{l'_{k+1} \notin \mathcal{L}_k} |\bar{\psi}_{(l'_{k+1}, t+1, H_k)}\rangle + |\bar{\psi}_{(0, t+1, H_k)}\rangle - |\bar{\psi}_{(0, t, H_k)}\rangle. \tag{34}$$

By substituting (34) into (31) for  $t < T$ , we arrive at

$$\begin{aligned} \sum_{l_k \in \mathcal{L}_k} \sum_{t=1}^T |\phi_{(l_k, t, H_k)}\rangle|^2 &= \left| \sum_{l_k \in \mathcal{L}_k} |\bar{\phi}_{(l_k, T, H_k)}\rangle + \sum_{t=1}^{T-1} \left( \sum_{l'_{k+1} \notin \mathcal{L}_k} |\bar{\psi}_{(l'_{k+1}, t+1, H_k)}\rangle + |\bar{\psi}_{(0, t+1, H_k)}\rangle - |\bar{\psi}_{(0, t, H_k)}\rangle \right) \right|^2 \\ &= \left| \sum_{l_k \in \mathcal{L}_k} |\bar{\phi}_{(l_k, T, H_k)}\rangle + \sum_{t=1}^{T-1} \sum_{l'_{k+1} \notin \mathcal{L}_k} |\bar{\psi}_{(l'_{k+1}, t+1, H_k)}\rangle + |\bar{\psi}_{(0, T, H_k)}\rangle - |\bar{\psi}_{(0, 1, H_k)}\rangle \right|^2 \end{aligned} \quad (35)$$

where for the sums over time in the last two terms only the states with maximal and minimal times remain.

Given that  $k < N$  and all parties must have measured by the end of the protocol, it must be the case that  $|\bar{\phi}_{(l_k, T, H_k)}\rangle = 0$  and  $|\bar{\psi}_{(0, T, H_k)}\rangle = 0$ . Also as  $k \geq 1$  it must be the case that  $|\bar{\psi}_{(0, 1, H_k)}\rangle = 0$  and  $|\bar{\psi}_{(l'_{k+1}, 1, H_k)}\rangle = 0$ , as these states are just before the first measurement and hence must have no history. Using these results in equation (35) and setting  $t' = t + 1$ , we obtain

$$\sum_{l_k \in \mathcal{L}_k} \sum_{t=1}^T |\phi_{(l_k, t, H_k)}\rangle|^2 = \left| \sum_{t'=1}^T \sum_{l'_{k+1} \notin \mathcal{L}_k} |\bar{\psi}_{(l'_{k+1}, t', H_k)}\rangle \right|^2. \quad (36)$$

Finally, using Lemma 1 and unitarity we arrive at

$$\begin{aligned} \sum_{l_k \in \mathcal{L}_k} \sum_{t=1}^T |\phi_{(l_k, t, H_k)}\rangle|^2 &= \sum_{t'=1}^T \sum_{l'_{k+1} \notin \mathcal{L}_k} \left| |\bar{\psi}_{(l'_{k+1}, t', H_k)}\rangle \right|^2 \\ &= \sum_{t'=1}^T \sum_{l'_{k+1} \notin \mathcal{L}_k} \left| |\psi_{(l'_{k+1}, t', H_k)}\rangle \right|^2 \end{aligned} \quad (37)$$

as required.

**Result 5** *We will now show that the results of the quantum protocol can be replicated by a causal process. In particular*

$$\begin{aligned} p(\vec{a}|\vec{x}) &= |(|\vec{a}\rangle \langle \vec{a}| \otimes I)U|0\rangle|^2 = \\ &= \sum_{l_1 \notin \mathcal{L}_0} \sum_{l_2 \notin \mathcal{L}_1} \dots \sum_{l_N \notin \mathcal{L}_{N-1}} p_1(l_1|H_0)p_1(a_{l_1}|H_0, x_{l_1})p_2(l_2|H_1)p_2(a_{l_2}|H_1, x_{l_2})\dots p_N(l_N|H_{N-1})p_N(a_{l_N}|H_{N-1}, x_{l_N}) \end{aligned} \quad (38)$$

and as such, the outcome statistics  $p(\vec{a}|\vec{x})$  cannot violate a causal inequality.

Proof: Firstly, substituting definitions 4 and 5 into the causal model (1), and then using Result 1, we can re-write the probability distribution for the entire causal model as

$$\begin{aligned} p(\vec{a}|\vec{x}) &= \sum_{l_1 \notin \mathcal{L}_0} \sum_{l_2 \notin \mathcal{L}_1} \dots \sum_{l_N \notin \mathcal{L}_{N-1}} \frac{\sum_{t_1=1}^T |\phi_{(l_1, t_1, H_1)}\rangle|^2}{\sum_{l'_1 \notin \mathcal{L}_0} \sum_{t'_1=1}^T |\psi_{(l'_1, t'_1, H_0)}\rangle|^2} \frac{\sum_{t_2=1}^T |\phi_{(l_2, t_2, H_2)}\rangle|^2}{\sum_{l'_2 \notin \mathcal{L}_1} \sum_{t'_2=1}^T |\psi_{(l'_2, t'_2, H_1)}\rangle|^2} \dots \\ &\dots \frac{\sum_{t_N=1}^T |\phi_{(l_N, t_N, H_N)}\rangle|^2}{\sum_{l'_N \notin \mathcal{L}_{N-1}} \sum_{t'_N=1}^T |\psi_{(l'_N, t'_N, H_{N-1})}\rangle|^2} \end{aligned} \quad (39)$$

Let us begin by performing a simple reshuffling of (39)'s numerators and denominators, by writing the denominator of the term associated to causal order stage  $k$  as the denominator of the term associated to  $k - 1$ .

$$\begin{aligned} p(\vec{a}|\vec{x}) &= \frac{1}{\sum_{l'_1 \notin \mathcal{L}_0} \sum_{t'_1=1}^T |\psi_{(l'_1, t'_1, H_0)}\rangle|^2} \sum_{l_1 \notin \mathcal{L}_0} \sum_{l_2 \notin \mathcal{L}_1} \dots \sum_{l_N \notin \mathcal{L}_{N-1}} \frac{\sum_{t_1=1}^T |\phi_{(l_1, t_1, H_1)}\rangle|^2}{\sum_{l'_2 \notin \mathcal{L}_1} \sum_{t'_2=1}^T |\psi_{(l'_2, t'_2, H_1)}\rangle|^2} \frac{\sum_{t_2=1}^T |\phi_{(l_2, t_2, H_2)}\rangle|^2}{\sum_{l'_3 \notin \mathcal{L}_2} \sum_{t'_3=1}^T |\psi_{(l'_3, t'_3, H_2)}\rangle|^2} \dots \\ &\dots \frac{\sum_{t_{k-1}=1}^T |\phi_{(l_{k-1}, t_{k-1}, H_{k-1})}\rangle|^2}{\sum_{l'_k \notin \mathcal{L}_{k-1}} \sum_{t'_k=1}^T |\psi_{(l'_k, t'_k, H_{k-1})}\rangle|^2} \dots \frac{\sum_{t_N=1}^T |\phi_{(l_N, t_N, H_N)}\rangle|^2}{\sum_{l'_N \notin \mathcal{L}_{N-1}} \sum_{t'_N=1}^T |\psi_{(l'_N, t'_N, H_{N-1})}\rangle|^2} \end{aligned} \quad (40)$$



by using Result 2 we have

$$p(\vec{a}|\vec{x}) = \sum_{l_1 \notin \mathcal{L}_0} \sum_{l_2 \notin \mathcal{L}_1} \dots \sum_{l_N \notin \mathcal{L}_{N-1}} \frac{\sum_{t_1=1}^T |\langle \phi_{(l_1, t_1, H_1)} \rangle|^2}{\sum_{l'_2 \notin \mathcal{L}_1} \sum_{t'_2=1}^T |\langle \psi_{(l'_2, t'_2, H_1)} \rangle|^2} \frac{\sum_{t_2=1}^T |\langle \phi_{(l_2, t_2, H_2)} \rangle|^2}{\sum_{l'_3 \notin \mathcal{L}_2} \sum_{t'_3=1}^T |\langle \psi_{(l'_3, t'_3, H_2)} \rangle|^2} \dots \sum_{t_N=1}^T |\langle \phi_{(l_N, t_N, H_N)} \rangle|^2 \quad (41)$$

now note that we can rewrite the leftmost sum as

$$\sum_{l_1 \notin \mathcal{L}_0} = \sum_{\mathcal{L}_1} \sum_{l_1 \in \mathcal{L}_1}, \quad (42)$$

where the sum over  $\mathcal{L}_1$  is over all singleton sets  $\{l_1\}$  (and hence has  $N$  terms), and the subsequent sum over  $l_1 \in \mathcal{L}_1$  contains just a single term.

We can use this to rewrite the probability distribution as

$$p(\vec{a}|\vec{x}) = \sum_{\mathcal{L}_1} \frac{\sum_{l_1 \in \mathcal{L}_1} \sum_{t_1=1}^T |\langle \phi_{(l_1, t_1, H_1)} \rangle|^2}{\sum_{l'_2 \notin \mathcal{L}_1} \sum_{t'_2=1}^T |\langle \psi_{(l'_2, t'_2, H_1)} \rangle|^2} \sum_{l_2 \notin \mathcal{L}_1} \dots \sum_{l_N \notin \mathcal{L}_{N-1}} \frac{\sum_{t_2=1}^T |\langle \phi_{(l_2, t_2, H_2)} \rangle|^2}{\sum_{l'_3 \notin \mathcal{L}_2} \sum_{t'_3=1}^T |\langle \psi_{(l'_3, t'_3, H_2)} \rangle|^2} \dots \sum_{t_N=1}^T |\langle \phi_{(l_N, t_N, H_N)} \rangle|^2 \quad (43)$$

where we have used the fact that the first numerator and denominator do not depend on  $\{l_2, \dots, l_N\}$ . By application of Result 4 this is just

$$p(\vec{a}|\vec{x}) = \sum_{\mathcal{L}_1} \sum_{l_2 \notin \mathcal{L}_1} \dots \sum_{l_N \notin \mathcal{L}_{N-1}} \frac{\sum_{t_2=1}^T |\langle \phi_{(l_2, t_2, H_2)} \rangle|^2}{\sum_{l'_3 \notin \mathcal{L}_2} \sum_{t'_3=1}^T |\langle \psi_{(l'_3, t'_3, H_2)} \rangle|^2} \dots \sum_{t_N=1}^T |\langle \phi_{(l_N, t_N, H_N)} \rangle|^2 \quad (44)$$

we can iterate the same process again using

$$\sum_{\mathcal{L}_1} \sum_{l_2 \notin \mathcal{L}_1} = \sum_{\mathcal{L}_2} \sum_{l_2 \in \mathcal{L}_2}. \quad (45)$$

The left-hand side corresponds to first picking  $l_1$  (with  $N$  possibilities) and then picking a different  $l_2$  ( $N-1$  possibilities), whereas the right-hand side corresponds to first picking a pair of distinct labs  $\mathcal{L}_2$  (with  $N(N-1)/2$  possibilities) and then picking which of them was last (2 possibilities). This gives

$$p(\vec{a}|\vec{x}) = \sum_{\mathcal{L}_2} \sum_{l_2 \in \mathcal{L}_2} \dots \sum_{l_N \notin \mathcal{L}_{N-1}} \frac{\sum_{t_2=1}^T |\langle \phi_{(l_2, t_2, H_2)} \rangle|^2}{\sum_{l'_3 \notin \mathcal{L}_2} \sum_{t'_3=1}^T |\langle \psi_{(l'_3, t'_3, H_2)} \rangle|^2} \dots \sum_{t_N=1}^T |\langle \phi_{(l_N, t_N, H_N)} \rangle|^2 \quad (46)$$

which is just

$$p(\vec{a}|\vec{x}) = \sum_{\mathcal{L}_2} \frac{\sum_{l_2 \in \mathcal{L}_2} \sum_{t_2=1}^T |\langle \phi_{(l_2, t_2, H_2)} \rangle|^2}{\sum_{l'_3 \notin \mathcal{L}_2} \sum_{t'_3=1}^T |\langle \psi_{(l'_3, t'_3, H_2)} \rangle|^2} \sum_{l_3 \notin \mathcal{L}_2} \dots \sum_{l_N \notin \mathcal{L}_{N-1}} \frac{\sum_{t_3=1}^T |\langle \phi_{(l_3, t_3, H_3)} \rangle|^2}{\sum_{l'_4 \notin \mathcal{L}_3} \sum_{t'_4=1}^T |\langle \psi_{(l'_4, t'_4, H_3)} \rangle|^2} \dots \sum_{t_N=1}^T |\langle \phi_{(l_N, t_N, H_N)} \rangle|^2 \quad (47)$$

application of Result 4 leads to another cancellation, so that we may write now

$$p(\vec{a}|\vec{x}) = \sum_{\mathcal{L}_2} \sum_{l_3 \notin \mathcal{L}_2} \dots \sum_{l_N \notin \mathcal{L}_{N-1}} \frac{\sum_{t_3=1}^T |\langle \phi_{(l_3, t_3, H_3)} \rangle|^2}{\sum_{l'_4 \notin \mathcal{L}_3} \sum_{t'_4=1}^T |\langle \psi_{(l'_4, t'_4, H_3)} \rangle|^2} \dots \sum_{t_N=1}^T |\langle \phi_{(l_N, t_N, H_N)} \rangle|^2 \quad (48)$$

We can then iterate this process by applying the general result that

$$\sum_{\mathcal{L}_k} \sum_{l_{k+1} \notin \mathcal{L}_k} = \sum_{\mathcal{L}_{k+1}} \sum_{l_{k+1} \in \mathcal{L}_{k+1}}, \quad (49)$$

and cancelling one of the numerators and denominators using Result 4 until we are left with the final term,

$$p(\vec{a}|\vec{x}) = \sum_{\mathcal{L}_N} \sum_{l_n \in \mathcal{L}_N} \sum_{t_N=1}^T |\langle \phi_{(l_N, t_N, H_N)} \rangle|^2 \quad (50)$$

the summation  $\sum_{\mathcal{L}_N} = 1$ , as the only term corresponds to  $\mathcal{L}_N = \{1, 2, \dots, N\}$ . Application of Result 3 then shows that this causal model indeed reproduces the quantum probabilities, i.e. that

$$p(\vec{a}|\vec{x}) = |(\vec{a} \langle \vec{a} | \otimes I) \mathcal{U} | 0 \rangle|^2 \quad (51)$$

as desired.

### III. EXAMPLE

We now give an example of how our results apply in practice, based on the quantum switch [1]. This involves using a quantum control to determine the order in which two operations are applied to another quantum system. The switch can be modelled in number of different ways (e.g. as a process matrix that exhibits causal non-separability [3]) but here the basic idea is to prepare a superposition state of the form

$$\frac{1}{\sqrt{2}} \left( |1\rangle_c \otimes U_A U_B |0\rangle_{sfr} + |2\rangle_c \otimes U_B U_A |0\rangle_{sfr} \right) \quad (52)$$

where  $U_A$  and  $U_B$  are unitary transformations by Alice and Bob (representing their measurements). If a third party, Charlie, measures the control in a basis consisting of superpositions of  $|1\rangle$  and  $|2\rangle$  this will introduce interference between the two causal orders in which either Alice or Bob goes first. It has already been shown that this simple setup cannot be used to violate a causal inequality [15, 21]. However, it is instructive to see how it fits into our framework.

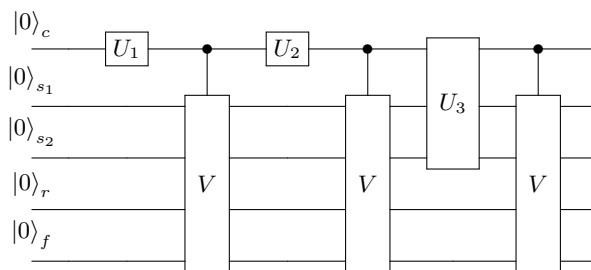


FIG. 4. Realisation of the quantum switch in our framework through a quantum circuit.

Because parties cannot directly measure the control in our framework, we transfer the state of the control into the system before Charlie's measurement, and split the system into two qubits to facilitate this. Overall, the circuit we consider is shown in figure 4, where

$$\begin{aligned} U_1 |0\rangle_c &= \frac{1}{\sqrt{2}} (|1\rangle_c + |2\rangle_c), \\ U_2 |1\rangle_c &= |2\rangle_c \\ U_2 |2\rangle_c &= |1\rangle_c \\ U_3 |1\rangle_c |\psi\rangle_{s_1} |0\rangle_{s_2} &= |3\rangle_c |0\rangle_{s_1} |\psi\rangle_{s_2}, \\ U_3 |2\rangle_c |\psi\rangle_{s_1} |0\rangle_{s_2} &= |3\rangle_c |1\rangle_{s_1} |\psi\rangle_{s_2}, \end{aligned} \quad (53)$$

and  $V$  is as given in equation 4 of the main body text.

By considering the outcome statistics generated by this switch setup, we find that they differ from those which would be obtained from an equal mixture of the causal orders  $A \rightarrow B \rightarrow C$  and  $B \rightarrow A \rightarrow C$ , due to the presence of interference.

We proceed with an explicit calculation for the setup in figure 4. We assume that all parties have two possible measurements, hence their input variables  $x, y, z$  are bits. When their input bit is zero, they measure the first part of the system in the computational basis and output the result in  $a, b, c$ . When their input bit is one, they instead measure the first part of the system in the Fourier basis (composed of the states  $|\pm\rangle = \frac{1}{\sqrt{2}} (|0\rangle \pm |1\rangle)$ ), and output zero if they obtain the state  $|+\rangle$  and one if they obtain the state  $|-\rangle$ . All of these measurements are implemented via unitary operations between the system and result register. e.g.

$$V_{s_1, r_1}(x_1 = 1) = |+\rangle \langle +|_{s_1} \otimes I_{r_1} + |-\rangle \langle -|_{s_1} \otimes (|0\rangle \langle 1|_{r_1} + |1\rangle \langle 0|_{r_1}) \quad (54)$$

Consider the case where the input variables are  $x = 0, y = 1, z = 1$ . After some calculation, we find the state at

the end of the protocol to be

$$\begin{aligned}
|3\rangle_c & \left( |+\rangle_{s_1} \left( \frac{1}{2\sqrt{2}} |+\rangle_{s_2} + \frac{1}{4} |0\rangle_{s_2} \right) |000\rangle_r + |-\rangle_{s_1} \left( \frac{1}{4} |0\rangle_{s_2} - \frac{1}{2\sqrt{2}} |+\rangle_{s_2} \right) |001\rangle_r \right. \\
& + |+\rangle_{s_1} \left( \frac{1}{2\sqrt{2}} |-\rangle_{s_2} + \frac{1}{4} |0\rangle_{s_2} \right) |010\rangle_r + |-\rangle_{s_1} \left( \frac{1}{4} |0\rangle_{s_2} - \frac{1}{2\sqrt{2}} |-\rangle_{s_2} \right) |011\rangle_r \\
& \left. + \frac{1}{4} |+\rangle_{s_1} |1\rangle_{s_2} |100\rangle_r + \frac{1}{4} |-\rangle_{s_1} |1\rangle_{s_2} |101\rangle_r - \frac{1}{4} |+\rangle_{s_1} |1\rangle_{s_2} |110\rangle_r - \frac{1}{4} |-\rangle_{s_1} |1\rangle_{s_2} |111\rangle_r \right) |111\rangle_f, \quad (55)
\end{aligned}$$

where we adopt the convention that  $|000\rangle_r = |a=0, b=0, c=0\rangle_r$ , et cetera. The probabilities to observe different outcomes in this measurement setting can then be obtained from this state. For example,  $p(000|011) = |\frac{1}{2\sqrt{2}} |+\rangle_{s_1} |+\rangle_{s_2} + \frac{1}{4} |+\rangle_{s_1} |0\rangle_{s_2}|^2 = 5/16$ . Such probabilities notably involve interference between different causal orders. In particular, they differ from those which would be obtained in the naive classical case, in which we first flip a coin to determine which of the two causal orders we will place ourselves in, and then perform the measurements in this causal order. We now calculate this ‘naive causal’ probability  $p^{\text{nc}}(000|011)$ . One half of the time, when we are in the causal order  $A \rightarrow B \rightarrow C$ , Alice measures 0 with certainty and Bob, and Charlie have each a 50 : 50 chance to measure either 0 or 1. The other half of the time, we are in the causal order  $B \rightarrow A \rightarrow C$  all parties have a 50 : 50 chance to measure either 0 or 1 (since Bob’s measurement in the Fourier basis, which occurs first, now makes Alice completely uncertain of her outcome). Putting this all together we find  $p^{\text{nc}}(000|011) = \frac{1}{2} \times 1 \times \frac{1}{2} \times \frac{1}{2} + \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} = 3/16 \neq p(000|011)$ .

Nevertheless, our results show that we *can* find some classical causal model which generates the same outcome distribution  $p(abc|xyz)$  as the quantum case. Let’s do this explicitly, to see how our proof translates in practice.

We find by direct substitution into the definitions 4, and 5 in the main body that:

$$\begin{aligned}
p_1(l_1 = \text{Alice}|H_0) &= 1/2 \\
p_1(l_1 = \text{Bob}|H_0) &= 1/2 \\
p_2(l_2 = \text{Bob}|H_1 = (1, 0, 0)) &= 1 \\
p_2(l_2 = \text{Alice}|H_1 = (2, 0, 1)) &= 1 \\
p_3(l_3 = \text{Charlie}|H_2 = ((1, 0, 0), (2, 0, 1))) &= 1 \\
p_3(l_3 = \text{Charlie}|H_2 = ((2, 0, 1), (1, 0, 0))) &= 1 \\
p_1(a = 0|H_0, x = 0) &= 1 \\
p_1(b = 0|H_0, y = 1) &= 1/2 \\
p_2(a = 0|H_1 = (1, 0, 0), x = 0) &= 1/2 \\
p_2(b = 0|H_1 = (2, 0, 1), y = 1) &= 1/2
\end{aligned} \quad (56)$$

which are all the same as the naive classical case. However, the results-type probability for Charlie differs from the naive case. In particular we find

$$\begin{aligned}
p_3(c = 0|H_2 = ((1, 0, 0), (2, 0, 1), z = 1)) &= \frac{5}{6} \\
p_3(c = 0|H_2 = ((2, 0, 1), (1, 0, 0), z = 1)) &= \frac{5}{6}.
\end{aligned} \quad (57)$$

Despite the ordering of the history for the classical protocol being different in these two cases, the quantum calculation given by definition 5 is the same for both (as it only depends on the flags raised and results obtained before Charlie measures). This leads to interference between the two causal orders of  $A$  and  $B$  in  $|\phi_{(l_3=\text{Charlie}, 3, H_2)}\rangle$ .

This alternative classical procedure which emulates the quantum experiment therefore gives  $p^{\text{ac}}(000|011) = \frac{1}{2} \times \frac{1}{2} \times \frac{5}{6} + \frac{1}{2} \times \frac{1}{2} \times \frac{5}{6} = 5/16$  as desired. Although we have focused on only one probability here, the same method can be used to generate a full classical strategy which replicates the quantum experiment for all input and output choices.

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- [32] Here, we summed from  $t = 1$  to  $T$ , but we could have equivalently chosen  $t = k$  to  $T - (N - k)$ , and only went with the former to make the subsequent notation easier to read, at the cost of including 0 amplitude states in our probability definition.
- [33] Nicolas Gisin, Jean-Daniel Bancal, Yu Cai, Patrick Remy, Armin Tavakoli, Emmanuel Zambrini Cruzeiro, Sandu Popescu, Nicolas Brunner. Constraints on nonlocality in networks from no-signaling and independence. *Nature Communications*, 11(1):2378, 2020
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