Revisiting optimal eavesdropping in quantum cryptography:
Optimal interaction is unique up to rotation of the underlying basis

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A general framework of optimal eavesdropping on BB84 protocol was provided by Fuchs \textit{et al}. [Phys. Rev. A, 1997]. An upper bound on mutual information was derived, which could be achieved by a specific type of interaction and the corresponding measurement. However, uniqueness of optimal interaction was posed as an unsolved problem there and it has remained open for almost two decades now. In this paper, we solve this open problem and establish the uniqueness of optimal interaction up to rotation. The specific choice of optimal interaction by Fuchs \textit{et al}. is shown to be a special case of the form derived in our work.

I. INTRODUCTION

Symmetric key cryptography requires a secret key to be shared or distributed between the sender (say, Alice) and the receiver (say, Bob). The security of classical key distribution is based on hardness assumptions for solving certain computational problems. This gives security against computationally bounded adversary in the classical domain, but fails to guarantee security against quantum attacks. Quantum key distribution (QKD) is based on the principles of quantum mechanics. To encode classical bits, QKD uses quantum states which the attacker (say, Eve) cannot measure without creating disturbance detectable by Bob. QKD protocol does not require any computation complexity assumption and is provably secure against both classical as well as quantum adversaries.

The first and possibly the most celebrated QKD protocol is BB84 [1]. The protocol relies on the use of orthogonal states from one of the two conjugate bases, say, $x$-$y$ and $u$-$v$, to encode a bit-string in qubits (e.g., polarized photons). Alice randomly selects one of the two bases and encodes 0 and 1 respectively by a qubit prepared in one of the two states in each base. Say, Alice encodes 0 to $|x\rangle$ or $|u\rangle$, and 1 to $|y\rangle$ or $|v\rangle$, depending on the chosen basis. When Bob receives a state from Alice, he randomly selects a basis $x$-$y$ or $u$-$v$ and makes a measurement. Once the measurement is done for all the received qubits, Alice and Bob publicly announce the sequence of bases used by them and discard the bits where the bases do not match. The resulting bit string, followed by error correction and privacy amplification, becomes the common secret key. However, presence of an eavesdropper may disturb the state of a qubit sent by Alice for which Bob may get a wrong result even if the corresponding bases of measurement between Alice and Bob match. To overcome this problem, Alice and Bob sacrifice some of the bits by comparing their values publicly.

Fuchs \textit{et al}. [2] provided a general framework of optimal eavesdropping on BB84 protocol. They derived an upper bound on mutual information, described a specific type of interaction and the corresponding measurement that achieves the bound. They finally explained an optimal strategy for Eve in interpreting her measurement. However, the optimal interaction described there was a specific choice and the uniqueness of the optimal interaction was left as an open problem. They commented: “\textit{It is easy to check that the solution here is correct, but the extent to which it is unique aside from trivial changes of basis and of phase remains unknown.}”

Interestingly, this problem has been open for last two decades. In this paper, we solve this open problem and establish the uniqueness up to rotation of the underlying basis. We characterize the classes of interaction that can achieve the already-existing optimal bound given by [2]. We have shown that the choice of optimal interaction in [2] is a special case of the generalized form provided by us. We also explicitly show the corresponding optimal measurement by Eve.

Note that Fuchs \textit{et al}. [2] made an intelligent guess to arrive at the expression for optimal interaction. On the other hand, in this paper, we explicitly derive the general form of the expression of any possible optimal interaction. See Sec. V for a more elaborate discussion on this issue.

The content of this paper is organized as follows. Section II explains basic terminologies used for optimal eavesdropping introduced in [2]. Section III contains summary of certain results from [2] which are relevant to our work. Our results are explained in Sec. IV. The remaining portion discusses the connection of our results with [2] followed by a conclusion.

II. PRELIMINARIES

Alice and Bob want to share a secret key using BB84 protocol. Alice randomly chooses a basis from $\mathcal{B}_{xy} = \{|x\rangle, |y\rangle\}$ and $\mathcal{B}_{uv} = \{|u\rangle, |v\rangle\}$, where

$$|x\rangle = \frac{1}{\sqrt{2}} (|u\rangle + |v\rangle), \quad |y\rangle = \frac{1}{\sqrt{2}} (|u\rangle - |v\rangle), \quad (1)$$
i.e., the bases are conjugate to each other.  

Alice encodes her key-bits, each as a polarized photon, and sends it to Bob. Suppose, an eavesdropper Eve interferes the communication while she lets a probe interact unitarily with the qubit sent by Alice.

Suppose Alice has chosen a signal, say, \(|x\rangle\) (corresponding density operator being \(\rho_x^A = |x\rangle \langle x|\)), in the basis \(\mathcal{B}_{xy}\). Eve lets a probe, initially in state \(|\psi_0\rangle\) (corresponding density operator \(\rho_0^E = |\psi_0\rangle \langle \psi_0|\)), interact unitarily (realized by a unitary operator \(U\)) with the qubit sent by Alice. The post-interaction joint state \(|X\rangle\) between Alice and Eve, which is an entangled state of the probe of Eve and the photon sent by Alice, is realized by

\[
|x\rangle \otimes |\psi_0\rangle \xrightarrow{U} |X\rangle.
\]

Bob receives a simple mixture of the two basis vectors (here \(\mathcal{B}_{xy}\)) chosen by Alice, i.e., Bob’s density matrix is always diagonal in the basis chosen by Alice. Thus, Schmidt decomposition of the post-interaction joint state \(|X\rangle\) must be of the form

\[
|X\rangle = \sqrt{\alpha} |x\rangle |\xi_x\rangle + \sqrt{1-\alpha} |y\rangle |\xi_y\rangle,
\]

such that

\[
|\xi_x\rangle \perp |\xi_y\rangle,
\]

where \(|\xi_x\rangle, |\xi_y\rangle\) are component of Eve’s part of the joint state after the interaction.

Similarly, when Alice sends \(|y\rangle\), the post-interaction state \(|Y\rangle\) must be of the form

\[
|Y\rangle = \sqrt{\beta} |y\rangle |\xi_y\rangle + \sqrt{1-\beta} |x\rangle |\xi_x\rangle,
\]

such that

\[
|\xi_y\rangle \perp |\xi_x\rangle.
\]

The density operator for the post-interaction state \(|X\rangle\) is given by

\[
\rho^{AE}_x = |X\rangle \langle X| = U (\rho^A_x \otimes \rho^E_0) U^\dagger.
\]

Eve’s description of the system will be \(^2\)

\[
rho_x := \rho^E_x = \text{tr}_A (\rho^{AE}_x) = \text{tr}_A (|X\rangle \langle X|),
\]

where tr\(_A\) represents partial trace over Alice’s qubit.

Since the interaction is unitary, it follows from Eqs. (1, 4) that

\[
|X\rangle = \frac{1}{\sqrt{2}} (|U\rangle + |V\rangle), \quad |Y\rangle = \frac{1}{\sqrt{2}} (|U\rangle - |V\rangle).
\]

Before performing any measurement, Eve waits until Alice declares her choice of basis publicly. Eve’s measurement is considered to be a Positive Operator-Valued Measure (POVM) \(\{E_\lambda\}\) or \(\{F_\lambda\}\) depending on whether Alice’s choice is \(x\)-y or \(u\)-v basis. Note that the operators \(\{E_\lambda\}\) satisfy two properties \([3, 4]\): they are all non-negative definite, i.e.,

\[
\langle \gamma | E_\lambda | \gamma \rangle \geq 0, \quad \forall |\gamma\rangle,
\]

and satisfy the completeness relation

\[
\sum_\lambda E_\lambda = 1.
\]

Suppose, Alice sends a signal in \(x\)-y (or, \(u\)-v) basis with the prior probabilities \(p_x, p_y\) (or, \(p_u, p_v\)) respectively. Once Alice reveals her basis to be \(x\)-y, Eve uses a POVM \(\{E_\lambda\}\) to perform a measurement on her probe. Considering \(A, B, E\) as random variables corresponding to the signal sent by Alice, signal received by Bob, and, measurement outcome of Eve, the conditional probability of the various outcomes \(\lambda\) of that measurement is given by

\[
P_{\lambda x} := \text{Pr}[E = \lambda | A = x] = \text{tr} (\rho_x E_\lambda),
\]

\[
P_{\lambda y} := \text{Pr}[E = \lambda | A = y] = \text{tr} (\rho_y E_\lambda).
\]

The probability that Eve gets outcome \(\lambda\), when Alice uses \(x\)-y basis is thus

\[
q_{xy}(\lambda) := \text{Pr}[E = \lambda] = P_{\lambda x} p_x + P_{\lambda y} p_y.
\]

Looking at outcome \(\lambda\), Eve assigns a guess for the signal sent by Alice following some strategy. The posterior probability \(Q_{x\lambda}\) (or \(Q_{y\lambda}\)) of the event that Alice had sent \(x\) (or \(y\)) given that Eve has observed \(\lambda\) is given by Bayes’ theorem.

\[
Q_{x\lambda} := \text{Pr}[A = x | E = \lambda] = \frac{P_{\lambda x} p_x}{q_{xy}(\lambda)},
\]

\[
Q_{y\lambda} := \text{Pr}[A = y | E = \lambda] = \frac{P_{\lambda y} p_y}{q_{xy}(\lambda)}.
\]

A simple way that Eve can utilize these likelihoods is to perform a guess realized by the following function.

\[
\text{argmax} \{Q_{x\lambda}, Q_{y\lambda}\} = \begin{cases} x, & \text{if } Q_{x\lambda} > Q_{y\lambda}, \\ y, & \text{if } Q_{y\lambda} > Q_{x\lambda}. \end{cases}
\]

A convenient measure of Eve’s information gain for an outcome \(\lambda\), as proposed in \([2]\), is

\[
G_{xy}(\lambda) := |Q_{x\lambda} - Q_{y\lambda}|.
\]

On average, Eve’s information gain over all outcomes is

\[
G_{xy} := \sum_\lambda q_{xy}(\lambda) G_{xy}(\lambda) = \sum_\lambda |P_{\lambda x} p_x - P_{\lambda y} p_y|.
\]

In particular, for equiprobable signals,

\[
G_{xy} = \frac{1}{2} \sum_\lambda |P_{\lambda x} - P_{\lambda y}|.
\]

---

1 Note that a more common notation uses \(|0\rangle, |1\rangle, |+\rangle\) and \(|-\rangle\) instead of \(|x\rangle, |y\rangle, |u\rangle\) and \(|v\rangle\) respectively. However, we follow the same notations as in Fuchs et al. \([2]\) so that the connection to their work is easily visible.

2 Henceforth, we use the notation := to denote “defined as”.
A more sophisticated data processing by Eve is mutual information [5]. For equal prior, this is given by

$$I_{xy} := \ln 2 + \sum_{\lambda} q_{xy}(\lambda) (Q_{x\lambda} \ln Q_{x\lambda} + Q_{y\lambda} \ln Q_{y\lambda}).$$

Eve’s attempt to measure the probe creates disturbance to the signal sent by Alice which is detectable by Bob. For signal sent in $x$-$y$ basis, the disturbance incorporated by Eve could be described by

$$D_{xy} := \sum_{\lambda} q_{xy}(\lambda) d_{xy}(\lambda),$$

where, $d_{xy}(\lambda)$ is the avg error for Bob to read the signal sent by Alice while Eve detects $\lambda$. For equal prior,

$$d_{xy}(\lambda) := \frac{1}{2} (d_{\lambda x} + d_{\lambda y}),$$

where, $d_{\lambda x}$ is the error for Bob when Alice sends $x$ while Eve detects $\lambda$ (i.e., Bob reads $y$), i.e.,

$$d_{\lambda x} := \Pr[|B = y| (A = x, \mathcal{E} = \lambda)],$$

and $d_{\lambda y}$ is the error for Bob when Alice sends $y$ while Eve detects $\lambda$ (i.e., Bob reads $x$), i.e.,

$$d_{\lambda y} := \Pr[|B = x| (A = y, \mathcal{E} = \lambda)].$$

Clearly, $D_{xy}$ is the observable error rate of Bob to read the signal sent by Alice prepared in $x$-$y$ basis.

Similarly, one can define $G_{uv}, I_{uv}, D_{uv}$ while considering Alice’s signal was prepared in $u$-$v$ basis. We drop the subscripts $xy$ and $uv$, i.e., use $G, I$, when both the bases to be considered in discussion.

### III. SUMMARY OF OPTIMAL EAVESDROPPING BY FUCHS ET AL. [2]

Optimal eavesdropping means that an eavesdropper performs the interaction and the measurement in such a way that she can extract maximum information about the signal sent by Alice, ensuring that the disturbance at Bob’s end remains bounded by a suitable threshold. In the QKD literature, it is interpreted as maximizing the information gain by Eve or mutual information between Alice and Eve. For BB84 protocol, considering the interaction to be unitary and restricted to equal prior ($p_x = \frac{1}{2} = p_y$), Fuchs et al. [2] provided an upper bound on information gain and mutual information over all possible interaction-POVM pairs. A criterion to achieve the bounds was provided there. To show that these bounds are attainable, an interaction-POVM pair for unequal error rates and another for equal error rates were provided therein. These results are discussed briefly in this section. Since these results hold for equal prior, the subsequent sections follow the same assumption unless explicitly mentioned.

### A. Upper bounds on information gain ($G$) and mutual information ($I$)

For equal prior, Fuchs et al. [2] provided an upper bound on the information gain ($G$). This bound was used to provide an upper bound on the mutual information ($I$). A necessary and sufficient condition to achieve the bounds was given there. We recollect these results here.

**Proposition 1.** (An upper bound on information gain ($G$)) [2, Eqs. (23,24)]

$$G_{xy} \leq 2 \sqrt{D_{uv} (1 - D_{uv})},$$

$$G_{uv} \leq 2 \sqrt{D_{xy} (1 - D_{xy})}. \tag{9}$$

Moreover, for measurement outcome $\lambda$ of Eve, the bound on information gain [2, Eq. (20)] can be expressed by the following inequality

$$G_{xy}(\lambda) \leq 2 \sqrt{d_{uv}(\lambda) [1 - d_{uv}(\lambda)]}. \tag{11}$$

It interesting to note that while Eve’s information gain refers to signals sent in the $x$-$y$ basis, Bob’s error rate refers to signals sent in the $u$-$v$ basis and vice versa.

**Proposition 2.** (An Upper Bound on Mutual Information ($I$)) [2, Eqs. (31,32)]

$$I_{xy} \leq \frac{1}{2} \phi \left[2 \sqrt{D_{uv} (1 - D_{uv})}\right],$$

$$I_{uv} \leq \frac{1}{2} \phi \left[2 \sqrt{D_{xy} (1 - D_{xy})}\right], \tag{13}$$

where $\phi(z) = (1 + z) \ln (1 + z) + (1 - z) \ln (1 - z)$.

Subscripts emphasize that the mutual information and error rate refer to signals sent in two different bases.

**Proposition 3.** (Necessary and Sufficient Conditions to Achieve $G^*$) [2, Eqs. (38,39)]

The necessary and sufficient conditions for equality in Eq. (9) are

$$|V_{\lambda u}\rangle = \varepsilon\lambda \sqrt{\frac{D_{uv}}{1 - D_{uv}}} |U_{\lambda u}\rangle \tag{14}$$

and

$$|U_{\lambda u}\rangle = \varepsilon\lambda \sqrt{\frac{D_{uv}}{1 - D_{uv}}} |V_{\lambda u}\rangle, \tag{15}$$

where

$$\varepsilon\lambda = \pm 1 = \text{sgn}(Q_{x\lambda} - Q_{y\lambda}) \tag{16}\text{.}$$

$q^*$ denotes optimal (maximum) value for any quantity $q$. 

Since the bases $x$ and $v$, assuming that all inner products
attains the bound in Eq. (9) does the same in Eq. (12)
optimizes $x$ also the same as those in Proposition 3. That is to say, for
and sufficient conditions for equality in Eqs. (12,13) are
interaction states are
basis.

Thus, for a signal sent in $x$-y basis, an interaction-POVM pair that
be achieved simultaneously while fixing $D_{xy}$, $D_{uv}$ independently [2]. One of the conditions that must hold
to achieve the bounds in (12,13) [and therefore the bounds (9,10)] could
what basis was used by Alice for encoding. Both the

B. Description of the postinteraction states $|X\rangle, |Y\rangle$

Eve’s objective is to maximize $G$ or $I$, irrespective of
what basis was used by Alice for encoding. Both the
bounds (12,13) [and therefore the bounds (9,10)] could be achieved simultaneously while fixing $D_{xy}$, $D_{uv}$ independently [2]. One of the conditions that must hold
to achieve the bounds in $x$-y basis is the following [2, Eq. (33)]:

$$d_{\lambda u} = d_{\lambda v} = d_{uv}(\lambda) = D_{uv}, \ \forall \lambda.$$ 

A similar condition holds good for signals sent in $u$-$v$ basis.

Thus, for a signal sent in $x$-y basis, the Schmidt de-
composition of the postinteraction states are

$$|X\rangle = \sqrt{1-D_{xy}} |x\rangle |\xi_x\rangle + \sqrt{D_{xy}} |y\rangle |\xi_y\rangle,$$

$$|Y\rangle = \sqrt{1-D_{xy}} |y\rangle |\xi_y\rangle + \sqrt{D_{xy}} |x\rangle |\xi_x\rangle.$$ 

Assuming that all inner products $\langle \xi_i | \xi_j \rangle$ are real, the
restrictions (2,3) on $|\xi_i\rangle, |\xi_j\rangle$ becomes more restricted as

$$\{|\xi_x\rangle, |\xi_y\rangle\} \perp \{|\xi_0\rangle, |\xi_1\rangle\}.$$ 

Similarly, for a signal sent in $u$-$v$ basis, the post-
interaction states are

$$|U\rangle = \sqrt{1-D_{uv}} |u\rangle |\xi_u\rangle + \sqrt{D_{uv}} |v\rangle |\xi_v\rangle,$$

$$|V\rangle = \sqrt{1-D_{uv}} |v\rangle |\xi_v\rangle + \sqrt{D_{uv}} |u\rangle |\xi_u\rangle.$$ 

Since the bases $B_{xy}$ and $B_{uv}$ are conjugate to each other, we expect to get a relationship between $|\xi_i\rangle, |\xi_j\rangle$ in $u$-$v$

basis and those in $x$-y basis which is described below.

Similarly,

$$2\sqrt{1-D_{uv}}|\xi_u\rangle = \sqrt{1-D_{xy}}(|\xi_x\rangle + |\xi_y\rangle) + \sqrt{D_{xy}}(|\xi_x\rangle + |\xi_y\rangle),$$

$$2\sqrt{D_{uv}}|\xi_v\rangle = \sqrt{1-D_{xy}}(|\xi_x\rangle - |\xi_y\rangle) + \sqrt{D_{xy}}(|\xi_x\rangle - |\xi_y\rangle).$$ 

From the orthogonality relation (19), one can say that
Eve’s probe lives in a Hilbert space of dimension at most four,
and thus is taken to be made of 2 qubits (4 states). It is therefore convenient to introduce same bases ($x$-$y$ and $u$-$v$, used by Alice) for each of Eve’s qubits.

C. Optimal interaction to maximize $G, I$:
A specific choice

Any interaction, as described above, that leads to op-
timality (i.e., attains $G^*$ or $I^*$) could be chosen. In [2, Sec. III: Eqs. (50,51),] one such specific choice was made for unequal error rates, which was shown to be a cor-
rect choice (correct in the sense that the choice leads to optimality). Similarly, for equal error rates, another spe-
cific choice was made in [2, Sec. IV, Eq. (69).] However,
uniqueness of the choice was left as an open problem in [2, Sec. III, first paragraph].

1. For unequal error rates, i.e., $D_{xy} \neq D_{uv}$

Equations (50, 51) of [2, Sec. III] are restated here. Consider a canonical basis for Eve’s probe as $\{|E_0\rangle, |E_1\rangle, |E_2\rangle, |E_3\rangle\}$. Without loss of generality,

$$|E_0\rangle = |x\rangle |x\rangle, |E_1\rangle = |y\rangle |x\rangle, |E_2\rangle = |x\rangle |y\rangle, |E_3\rangle = |y\rangle |y\rangle.$$ 

To describe $|\xi_i\rangle, |\xi_j\rangle$, the work [2] considered an orthonor-
mal set, namely, the Bell Basis with respect to (w.r.t.) $x$-$y$, as follows.

$$|\Phi^\pm_{xy}\rangle := \frac{1}{\sqrt{2}} (|x\rangle |x\rangle \pm |y\rangle |y\rangle) = \frac{1}{\sqrt{2}} (|E_0\rangle \pm |E_3\rangle),$$

$$|\Psi^\pm_{xy}\rangle := \frac{1}{\sqrt{2}} (|x\rangle |y\rangle \pm |y\rangle |x\rangle) = \frac{1}{\sqrt{2}} (|E_2\rangle \pm |E_1\rangle).$$ 

In terms of the Bell basis vectors for Eve’s probe, the
interaction was chosen such that

$$|\xi_x\rangle = \sqrt{1-D_{uv}} |\Phi^+_{xy}\rangle + \sqrt{D_{uv}} |\Phi^-_{xy}\rangle,$$

$$|\xi_y\rangle = \sqrt{1-D_{uv}} |\Phi^+_{xy}\rangle - \sqrt{D_{uv}} |\Phi^-_{xy}\rangle,$$

$$|\xi_x\rangle = \sqrt{1-D_{uv}} |\Psi^+_{xy}\rangle - \sqrt{D_{uv}} |\Psi^-_{xy}\rangle,$$

$$|\xi_y\rangle = \sqrt{1-D_{uv}} |\Psi^+_{xy}\rangle + \sqrt{D_{uv}} |\Psi^-_{xy}\rangle.$$ 

The corresponding optimal POVM, as shown in [2, Eqs. (55,56)], is described below.

$$E_\lambda = |E_\lambda\rangle \langle E_\lambda|,$$
where
\[ |E_0\rangle = |\xi_0\rangle, \quad |E_1\rangle = |\xi_1\rangle, \quad |E_2\rangle = |\xi_2\rangle, \quad |E_3\rangle = |\xi_3\rangle. \quad (26) \]

Introducing new notations \( \mathcal{D}_{uv}, \mathcal{F}_{uv} \), we can write a closed form of \( |\xi_i\rangle, |\zeta_i\rangle \) as below.
\[
\begin{align*}
|\xi_x\rangle &= \mathcal{D}_{uv} |\xi_0\rangle + \mathcal{F}_{uv} |\xi_3\rangle, \\
|\xi_y\rangle &= \mathcal{D}_{uv} |\xi_0\rangle + \mathcal{F}_{uv} |\xi_2\rangle, \\
|\zeta_x\rangle &= \mathcal{F}_{uv} |\xi_2\rangle + \mathcal{D}_{uv} |\xi_1\rangle, \\
|\zeta_y\rangle &= \mathcal{D}_{uv} |\xi_2\rangle + \mathcal{F}_{uv} |\xi_1\rangle,
\end{align*}
\]
(27)
where
\[
\begin{align*}
\mathcal{D}_{uv} &= \frac{\sqrt{1 - D_{uv}} + \sqrt{D_{uv}}}{\sqrt{2}}, \\
\mathcal{F}_{uv} &= \frac{\sqrt{1 - D_{uv}} - \sqrt{D_{uv}}}{\sqrt{2}}.
\end{align*}
\] (28)
The following relations appear to be useful.
\[
\begin{align*}
\mathcal{D}_{uv} \mathcal{F}_{uv} &= \frac{1}{2} (1 - 2D_{uv}), \\
\mathcal{D}_{uv}^2 + \mathcal{F}_{uv}^2 &= 1, \\
\mathcal{D}_{uv}^2 - \mathcal{F}_{uv}^2 &= 2\sqrt{D_{uv}} (1 - D_{uv}).
\end{align*}
\] (29)
The above analysis works for a signal sent in \( x-y \) basis. Similar analysis holds for \( u-v \) basis as well.

2. For equal error rates, i.e., \( D_{xy} = D_{uv} = D \)

For equal error rates, [2, Sec. IV, Eq. (69)] comes up with another choice of \( |\xi_i\rangle, |\zeta_i\rangle \). We describe it as below.
\[
\begin{align*}
|\xi_x\rangle &= |x\rangle |x\rangle, \\
|\xi_y\rangle &= (\cos \alpha |x\rangle + \sin \alpha |y\rangle) |x\rangle, \\
|\zeta_x\rangle &= |x\rangle |y\rangle, \\
|\zeta_y\rangle &= (\cos \beta |x\rangle + \sin \beta |y\rangle) |y\rangle.
\end{align*}
\] (30)
Optimality of \( G \) (or \( I \)) is reached when
\[
\alpha = \beta \quad \text{and} \quad \sin \alpha = 2 \sqrt{D (1 - D)} = \mathcal{D}^2 - \mathcal{F}^2.
\]
Here, the notations \( \mathcal{D}, \mathcal{F} \) are analogous to \( \mathcal{D}_{uv}, \mathcal{F}_{uv} \) in Eq. (28) but for equal error rates, i.e., to consider \( D \) for the right hand side of Eq. (28).
Thus, the optimal interaction can be written as
\[
\begin{align*}
|\xi_x\rangle &= |\xi_0\rangle, \\
|\xi_y\rangle &= 2 \mathcal{D} \mathcal{F} |\xi_0\rangle + (\mathcal{D}^2 - \mathcal{F}^2) |\xi_1\rangle, \\
|\zeta_x\rangle &= |\xi_2\rangle, \\
|\zeta_y\rangle &= 2 \mathcal{D} \mathcal{F} |\xi_2\rangle + (\mathcal{D}^2 - \mathcal{F}^2) |\xi_3\rangle.
\end{align*}
\] (31)
However, the corresponding optimal POVM was not shown explicitly in [2], which we establish in Sec. IV C.

Although, both interactions (27,31) lead to optimality, the way they were proposed in [2] seems to be an intelligent guesswork. This leaves open a few interesting questions:

1. Instead of guessing an interaction and verifying its optimality, can one derive it from first principle?
2. Are there other possible optimal interactions than the two specific ones?
3. If so, is it possible to characterize them?

We address these questions in the following section.

IV. OUR RESULTS

In this section, we derive an expression for an interaction by Eve that leads to optimal information gain. Eventually, we show that the expression is unique in a fixed basis. Associated optimal POVMs are then identified.

Given an interaction, how to identify an optimal POVM is discussed in the following subsection.

A. Optimal measurement (POVM) to maximize information gain \( G \) for a given interaction

Let’s consider the problem below: given an interaction,
\[
\text{maximize } G_{xy} = \sum_\lambda |P_{\lambda x} p_x - P_{\lambda y} p_y| \]
over all POVMs \( \{E_\lambda\} \).

In [3], an optimal measurement for this maximization was derived. There, the maximization was done on Kolmogorov Variational Distance [3, Eq. (130)]. The calculation was performed in [3, Appendix (Sec. 7)], which shows that the optimal measurement corresponds to a Hermitian operator given by [3, Eq. (21)] and the optimal POVM consists of the projectors onto an orthonormal eigenbasis of that operator. We describe the result here with a proof in terms of maximizing \( G \). Note that this result is presented here for the sake of completeness and easy reference and we do not claim any contribution for this result.

**Lemma 1.** Given an interaction, an optimal POVM to attain maximum information gain consists of the eigoprojectors \( \{E_\lambda\} \) onto the orthonormal eigenbasis \( \{|\tilde{E}_\lambda\rangle\} \) that diagonalizes the Hermitian operator
\[
\tilde{\Gamma}_{xy} := p_x \rho_x - p_y \rho_y,
\] (32)
where \( \rho_x \), as defined in Eq. (5), is the partial trace (over Alice’s qubit) of the post-interaction state \( |X\rangle \). The maximum achievable information gain is \( \text{tr} |\tilde{\Gamma}_{xy}| \).

**Proof.** Given an interaction (i.e., the density operators \( \rho_x, \rho_y \) get fixed), the associated \( \tilde{\Gamma}_{xy} \) being Hermitian is diagonalizable by an orthonormal eigenbasis \( \{|\tilde{\gamma}_i\rangle\} \). Let the corresponding eigenvalues (all real) are \( \{\tilde{\gamma}_i\} \). Then,
over all POVMs \( \{ E_\lambda \} \),
\[
G_{xy} = \sum_\lambda |P_{x\lambda}p_x - P_{y\lambda}p_y|
\]
\[
= \sum_\lambda |p_x \text{tr} (\rho_x E_\lambda) - p_y \text{tr} (\rho_y E_\lambda)| , \text{ using Eqs. (7, 8)}
\]
\[
= \sum_\lambda | \text{tr} (\tilde{\Gamma}_{xy} E_\lambda) | , \text{ using Eq. (32)}
\]
\[
= \sum_\lambda \left| \sum_i \gamma_i \langle \gamma_i | E_\lambda | \gamma_i \rangle \right|
\]
\[
\leq \sum_\lambda \left| \sum_i |\gamma_i| \langle \gamma_i | E_\lambda | \gamma_i \rangle \right|
\]
\[
= \sum_i |\gamma_i| \langle \gamma_i | \sum_\lambda E_\lambda | \gamma_i \rangle
\]
\[
= \sum_i |\gamma_i| = \text{tr} |\tilde{\Gamma}_{xy}| .
\]

The upper bound could be achieved by some POVM \( \{ E_\lambda \} \) consisting of the projectors onto an orthonormal eigenbasis of \( \tilde{\Gamma}_{xy} \).

**Remark 1.** Since we consider equal prior probabilities here, analogous to Eq. (32), we define
\[
\Gamma_{xy} := \frac{1}{2} (\rho_x - \rho_y)
\]
and use it throughout the rest of the paper.

**Remark 2.** Given an interaction, a POVM optimal for \( G_{xy} \) may not necessarily be optimal for \( I_{xy} \) [2, 3]. However, for equal prior, once the bound \( \text{tr} |\tilde{\Gamma}_{xy}| \) of \( G_{xy} \) in Lemma 1 becomes equal to the upper bound \( \mathcal{D}_u^2 - \mathcal{D}_{uv}^2 \) of \( G_{xy} \) in Eq. (9), the interaction is called optimal. In that case, the interaction-POVM pair also attains the upper bound (12) of \( I_{xy} \).

**B. Optimal interaction to maximize information gain \( (G) \): A generic form of optimal \( |\xi_i \rangle, |\xi_j \rangle \)**

We use the following result for equal priors to find an expression of \( |\xi_i \rangle, |\xi_j \rangle \) for optimal interaction.

**Lemma 2.** Optimality conditions for \( G_{xy} \) ensure that each \( G_{xy}^*(\lambda) \) is equal to \( G_{xy}^* \) and the corresponding optimal value is given by
\[
G_{xy}^* = 2\sqrt{D_{uv} (1 - D_{uv})} = G_{xy}^* (\lambda) , \forall \lambda .
\]

**Proof.** For signal sent in \( x-y \) basis, the optimal information gain, by Eq. (9), is
\[
G_{xy}^* = 2\sqrt{D_{uv} (1 - D_{uv})} .
\]
By Eq. (11), for measurement outcome \( \lambda \) of Eve,
\[
G_{xy}^* (\lambda) = 2\sqrt{d_{uv}(\lambda) [1 - d_{uv}(\lambda)]}
\]
For optimality, the necessary and sufficient conditions in Proposition 3 must be satisfied. By [2, Eq. (33)], this requires
\[
d_{uv}(\lambda) = D_{uv}, \forall \lambda
\]
which ensures that the lemma is proved.

**Note 1.** Since we consider equal prior probabilities, we use the following working formula of \( G_{xy}^*(\lambda) \) while we derive the general form of an optimal interaction,
\[
G_{xy}^*(\lambda) = |Q_{x\lambda} - Q_{y\lambda}| = |P_{x\lambda} - P_{y\lambda}| / (P_{x\lambda} + P_{y\lambda}) . \tag{35}
\]

Here we describe an expression of \( P_{x\lambda}, P_{y\lambda} \) in terms of \( |\xi_i \rangle, |\xi_j \rangle \) and a POVM \( \{ E_\lambda \} \).

**Theorem 1.** Given the postinteraction sates (18), and a POVM \( \{ E_\lambda \}_{\lambda \in \{0,1,2,3\}} \),
\[
P_{x\lambda} = (1 - D_{xy}) |\xi_x | E_\lambda \rangle \langle E_\lambda | + D_{xy} |\xi_y | E_\lambda \rangle \langle E_\lambda | ,
\]
\[
P_{y\lambda} = (1 - D_{xy}) |\xi_y | E_\lambda \rangle \langle E_\lambda | + D_{xy} |\xi_x | E_\lambda \rangle \langle E_\lambda | . \tag{36}
\]

**Proof.** Using Eq. (18) in Eq. (5), we get,
\[
\rho_x = \text{Tr}_A (|X \rangle \langle X |) = (1 - D_{xy}) \tilde{\xi}_x + D_{xy} \tilde{\xi}_y , \tag{37}
\]
where
\[
\tilde{\xi}_x := |\xi_x \rangle \langle \xi_x | , \quad \tilde{\xi}_y := |\xi_y \rangle \langle \xi_y | .
\]
By Eq. (7),
\[
P_{x\lambda} = \text{Tr} (\rho_x E_\lambda) = (1 - D_{xy}) \text{Tr} (\tilde{\xi}_x E_\lambda) + D_{xy} \text{Tr} (\tilde{\xi}_y E_\lambda)
\]
\[
= (1 - D_{xy}) |\xi_x | E_\lambda \rangle \langle E_\lambda | + D_{xy} |\xi_y | E_\lambda \rangle \langle E_\lambda | .
\]
Similarly, we can derive an expression for \( P_{y\lambda} \).

We now have all the required pieces in place to derive the optimal interactions. First we gauge the difficulty of performing the derivation if we express the interaction vectors in canonical basis \( \{ |\xi_i \rangle \} \). We notice that the expressions (36) of \( P_{x\lambda}, P_{y\lambda} \) are dependent on the eigenvectors \( \{ E_\lambda \} \) for which we don’t have any easy formulation against an arbitrary interaction expressed in canonical basis. As we will see shortly, this blockage could be tackled if we express the interaction vectors \( |\xi_i \rangle, |\xi_j \rangle \) in the orthonormal eigenbasis of the associated Hermitian \( \tilde{\Gamma}_{xy} \).

Having understood this way of describing the interaction vectors, we start with a general form (39) of \( |\xi_i \rangle, |\xi_j \rangle \) expressed in the associated orthonormal eigenbasis \( \{ |E_\lambda \rangle \} \), while abiding by the orthogonality restriction (19). Subsequently, we plug-in the expression (39) of the interaction vectors into Eq. (36) to get the probabilities \( P_{x\lambda}, P_{y\lambda} \). Then we substitute these probabilities into Eq. (35) to get values of \( G_{xy}^*(\lambda) \). Finally, comparing these values with their optimal counterparts in Eq. (34), we derive the general form of an optimal interaction \( |\xi_i \rangle, |\xi_j \rangle \) realized in eigenbasis \( \{ |E_\lambda \rangle \} \).
This way of expressing interaction vectors not only helps us derive the optimal interactions, but, as we will see shortly, all the optimal interactions eventually lead to a unique expression.

**Theorem 2.** Let \(|E_\lambda\rangle\) be an orthonormal eigenbasis of \(\Gamma_{xy}\) associated with arbitrary interaction vectors \(|\xi_i\rangle, |\zeta_j\rangle\) in Eq. (18) of the postinteraction states while abiding by the orthogonality restriction (19). Then, for optimal interaction, the general form of \(|\xi_i\rangle, |\zeta_j\rangle\), described in that eigenbasis becomes

\[
|\xi_x\rangle = \mathcal{D}_{uv} |E_0\rangle + \mathcal{T}_{uv} |E_1\rangle,
|\xi_y\rangle = \mathcal{D}_{uv} |E_0\rangle + \mathcal{T}_{uv} |E_3\rangle,
|\zeta_x\rangle = \mathcal{D}_{uv} |E_2\rangle + \mathcal{T}_{uv} |E_3\rangle,
|\zeta_y\rangle = \mathcal{D}_{uv} |E_2\rangle + \mathcal{T}_{uv} |E_3\rangle,
\]

where \(\mathcal{D}_{uv}, \mathcal{T}_{uv}\) are as defined in Eq. (28).

**Proof.** First we need to fix an orthonormal basis to describe \(|\xi_i\rangle, |\zeta_j\rangle\) following restriction (19). For that purpose, there is no harm to choose the above eigenbasis to describe \(|\xi_i\rangle, |\zeta_j\rangle\). Orthogonality restriction (19) is automatically satisfied if we choose \(|\xi_i\rangle \in \text{span}\{ |E_0\rangle, |E_1\rangle\}\) and \(|\zeta_j\rangle \in \text{span}\{ |E_2\rangle, |E_3\rangle\}\). So the general form of \(|\xi_i\rangle, |\zeta_j\rangle\) becomes

\[
|\xi_x\rangle = \sqrt{\alpha} |E_0\rangle + \sqrt{1-\alpha} |E_1\rangle,
|\xi_y\rangle = \sqrt{\beta} |E_0\rangle + \sqrt{1-\beta} |E_1\rangle,
|\zeta_x\rangle = \sqrt{\mu} |E_2\rangle + \sqrt{1-\mu} |E_3\rangle,
|\zeta_y\rangle = \sqrt{\nu} |E_2\rangle + \sqrt{1-\nu} |E_3\rangle.
\]

Using this form of \(|\xi_i\rangle, |\zeta_j\rangle\) in Eq. (36), we find values of \(G_{xy}(\lambda)\) as shown in Table I.

By Lemma 2, for optimal \(G_{xy}\), the values of \(G_{xy}(\lambda)\) are all equal. Equating \(G_{xy}(0), G_{xy}(1)\) in Table I, we get,

\[
\alpha + \beta = 1, \quad G_{xy}(0) = G_{xy}(1) = |2\alpha - 1|.
\]

Similarly, equating \(G_{xy}(2), G_{xy}(3)\) in Table I, we get,

\[
\mu + \nu = 1, \quad G_{xy}(2) = G_{xy}(3) = |2\mu - 1|.
\]

Together, equating \(G_{xy}(0), G_{xy}(2)\), we get,

\[
\mu = \alpha, \quad \nu = \beta = 1 - \alpha.
\]

Thus,

\[
G_{xy}^*(0) = \mathcal{D}_{uv}^2 - \mathcal{T}_{uv}^2 = 2\mathcal{D}_{uv}^2 - 1 = |2\alpha - 1|
\]

gives rise to

\[
\sqrt{\alpha} = \mathcal{D}_{uv}, \quad \sqrt{1-\alpha} = \mathcal{T}_{uv}.
\]

Using Eqs. (41,40) in Eq. (39), we get a generic form for optimal \(|\xi_i\rangle, |\zeta_j\rangle\) as in Eq. (38).

Analogous to Eq. (38), a set of optimal interaction vectors exist in \(u-v\) basis.

The most interesting thing with the expression (38) of the optimal interaction vectors is that it has a unique form capturing all the optimal interactions while realized in the orthonormal eigenbasis of the associated \(\Gamma_{xy}\).

**Remark 3.** An optimal interaction for equal error rates could be described by an expression analogous to Eq. (38) while \(\mathcal{D}_{uv}, \mathcal{T}_{uv}\) are replaced by \(\mathcal{D}, \mathcal{T}\) respectively.

**Remark 4.** We can rewrite Eq. (38) as below.

\[
|\xi_x\rangle = \sqrt{1-D_{uv}} |E_0\rangle + \sqrt{D_{uv}} |E_1\rangle,
|\xi_y\rangle = \sqrt{1-D_{uv}} |E_0\rangle - \sqrt{D_{uv}} |E_1\rangle,
|\zeta_x\rangle = \sqrt{1-D_{uv}} |E_2\rangle + \sqrt{D_{uv}} |E_3\rangle,
|\zeta_y\rangle = \sqrt{1-D_{uv}} |E_2\rangle - \sqrt{D_{uv}} |E_3\rangle,
\]

where

\[
|\tilde{E}_0\rangle = \frac{1}{\sqrt{2}} (|E_0\rangle + |E_1\rangle), \quad |\tilde{E}_1\rangle = \frac{1}{\sqrt{2}} (|E_0\rangle - |E_1\rangle),
|\tilde{E}_2\rangle = \frac{1}{\sqrt{2}} (|E_2\rangle + |E_3\rangle), \quad |\tilde{E}_3\rangle = \frac{1}{\sqrt{2}} (|E_2\rangle - |E_3\rangle).
\]

is another orthonormal basis (called, Bell basis), written in terms of an optimal eigenbasis \(|E_\lambda\rangle\). Clearly, these form to describe \(|\xi_i\rangle, |\zeta_j\rangle\) is analogous to Eqs. (51) and (50), respectively, as in [2].

As we will see in the next subsections, expression (38) hides a family of optimal interactions via the eigenbasis \(|E_\lambda\rangle\) – we can unfold it once we identify the associated optimal POVMs. Since an optimal POVM corresponds to some \(\Gamma_{xy}\), we need to find the expression of \(\Gamma_{xy}\) realizing interactions (38).

**Theorem 3.** For an optimal interaction (38,18), and its optimal POVM \(|E_\lambda\rangle\),

\[
\Gamma_{xy} = \frac{1}{2} (\mathcal{D}_{uv}^2 - \mathcal{T}_{uv}^2) [(1-D_{xy})(|E_{00} - E_{11}|) + D_{xy} (|E_{22} - E_{33}|)],
\]

where \(E_{ij} := |E_i\rangle \langle E_j|\).

**Proof.** By Eq. (37) and its analogue for signal \(y\),

\[
2\Gamma_{xy} = \rho_x - \rho_y = (1-D_{xy}) (\hat{\xi}_x - \hat{\zeta}_y) + D_{xy} (\hat{\xi}_x - \hat{\zeta}_y).
\]

Using expressions of \(|\xi_i\rangle, |\zeta_j\rangle\) in Eq. (38), we get,

\[
\hat{\xi}_x = \mathcal{D}_{uv} E_{00} + \mathcal{T}_{uv} E_{11} + 2 \mathcal{D}_{uv} \mathcal{T}_{uv} (E_{01} + E_{10}),
\hat{\xi}_y = \mathcal{D}_{uv} E_{00} + \mathcal{T}_{uv} E_{11} + 2 \mathcal{D}_{uv} \mathcal{T}_{uv} (E_{01} + E_{10}),
\hat{\zeta}_x = \mathcal{D}_{uv} E_{22} + \mathcal{T}_{uv} E_{33} + 2 \mathcal{D}_{uv} \mathcal{T}_{uv} (E_{23} + E_{32}),
\hat{\zeta}_y = \mathcal{D}_{uv} E_{22} + \mathcal{T}_{uv} E_{33} + 2 \mathcal{D}_{uv} \mathcal{T}_{uv} (E_{23} + E_{32}),
\]

which leads to the desired form of \(\Gamma_{xy}\).

**Remark 5.** Clearly, \(\Gamma_{xy}\) in (44) is diagonalized by its eigenbasis while its eigenvalues are

\[
\gamma_0 = \frac{1}{2} (\mathcal{D}_{uv}^2 - \mathcal{T}_{uv}^2) (1-D_{xy}), \quad \gamma_1 = -\gamma_0,
\gamma_2 = \frac{1}{2} (\mathcal{D}_{uv}^2 - \mathcal{T}_{uv}^2) D_{xy}, \quad \gamma_3 = -\gamma_2.
\]
TABLE I: Values of $P_{\lambda x}, P_{\lambda y}, G_{xy}(\lambda)$ for the general form of $|\xi_i\rangle, |\zeta_j\rangle$ as in Eq. (39).

| $\lambda$ | $P_{\lambda x}$ | $P_{\lambda y}$ | $G_{xy}(\lambda) = \frac{|P_{\lambda x} - P_{\lambda y}|}{P_{\lambda x} + P_{\lambda y}}$ |
|-----------|----------------|----------------|--------------------------------------------------|
| 0         | $(1 - D_{xy})(\xi_x|E_0\rangle)^2 = (1 - D_{xy})\alpha$ | $(1 - D_{xy})(\xi_y|E_0\rangle)^2 = (1 - D_{xy})\beta$ | $|\alpha - \beta|/(\alpha + \beta)$ |
| 1         | $(1 - D_{xy})(\xi_x|E_1\rangle)^2 = (1 - D_{xy})(1 - \alpha)$ | $(1 - D_{xy})(\xi_y|E_1\rangle)^2 = (1 - D_{xy})(1 - \beta)$ | $|\beta - \alpha|/(1 - \alpha + 1 - \beta)$ |
| 2         | $D_{xy}(\xi_x|E_2\rangle)^2 = D_{xy}\mu$ | $D_{xy}(\xi_y|E_2\rangle)^2 = D_{xy}\nu$ | $|\mu - \nu|/(\mu + \nu)$ |
| 3         | $D_{xy}(\xi_x|E_3\rangle)^2 = D_{xy}(1 - \mu)$ | $D_{xy}(\xi_y|E_3\rangle)^2 = D_{xy}(1 - \nu)$ | $|\mu - \nu|/(1 - \mu + 1 - \nu)$ |

It is worth to note here that, for interactions (38), the optimal value $\mathcal{G}_{uv}^2 - \mathcal{G}_{uv}^2$ of $G_{xy}$ in Eq. (9) agrees with the upper bound $\sum_{\lambda} |\gamma_{\lambda}|$ of $G_{xy}$ in Lemma 1.

As a first step towards identifying the optimal POVMs hiding behind the interactions (38), we connect them with the known instances (27,31).

In Eq. (38), a mere replacement of the eigenbasis $\{|E_i\rangle\}$ by the canonical basis $\{|\xi_i\rangle\}$ leads to the interaction (27), except for a trivial permutation of the basis vectors. The corresponding $\Gamma_{xy}$ in Eq. (44) becomes

$$\Gamma_{xy} = \frac{1}{2}(\mathcal{G}_{uv}^2 - \mathcal{G}_{uv}^2)((1 - D_{xy})(\xi_{10} - \xi_{11}) + D_{xy}(\xi_{22} - \xi_{33})),$$

where $\xi_{ij}$ stands for $|\xi_i\rangle \langle \xi_i|$. Clearly, the canonical basis $\{|\lambda_i\rangle\}$ diagonalizes this $\Gamma_{xy}$ and therefore constitutes the optimal POVM (26) for the said interaction. The diagonalization worked due to orthonormality of the canonical basis.

Connecting Eq. (38) to the instance (31) is done in the following subsection.

C. Optimal POVM for the specific interaction for equal error rates ($D_{xy} = D_{uv} = D$) by Fuchs et al. [2]

For equal error rates, i.e., $D_{xy} = D_{uv} = D$, [2] described a choice of $|\xi_i\rangle, |\zeta_j\rangle$, that optimizes $I$ (and therefore $G$). For this optimal $|\xi_i\rangle, |\zeta_j\rangle$ as described in Eq. (31), we now derive the optimal POVM that was not shown in [2]. To see how Eq. (38) produces Eq. (31), one can simply compare the respective interaction vectors in each of these equations. The comparison gives rise to a set of vectors $\{|E_{\lambda}\rangle\}$, which constitutes an optimal POVM if it diagonalizes the corresponding $\Gamma_{xy}$.

**Theorem 4.** Consider a canonical basis for Eve as given in Eq. (23). For the optimal interaction (31), the optimal POVM $\{E_{\lambda}\}$ can be given by

$$E_{\lambda} = |E_{\lambda}\rangle \langle E_{\lambda}|,$$

where

$$|E_0\rangle = \mathcal{D}|\xi_0\rangle - \mathcal{D}|\xi_1\rangle, |E_1\rangle = \mathcal{D}|\xi_0\rangle + \mathcal{D}|\xi_1\rangle,$$

$$|E_2\rangle = \mathcal{D}|\xi_2\rangle - \mathcal{D}|\xi_3\rangle, |E_3\rangle = \mathcal{D}|\xi_2\rangle + \mathcal{D}|\xi_3\rangle. \quad (46)$$

**Proof.** Comparing a special form of $|\xi_i\rangle, |\zeta_j\rangle$ given by Eq. (31) and the general form of $|\xi_i\rangle, |\zeta_j\rangle$ described in Eq. (38) but for equal error rates, we get

$$\mathcal{D}|E_0\rangle + \mathcal{D}|E_1\rangle = |E_0\rangle,$$

$$\mathcal{D}|E_0\rangle + \mathcal{D}|E_1\rangle = 2\mathcal{D}|E_0\rangle + (\mathcal{G}^2 - \mathcal{G}^2)|E_1\rangle. \quad (47)$$

Solving for $|E_0\rangle$ and $|E_1\rangle$, one should arrive at the first two expressions of Eq. (46). The remaining two expressions in Eq. (46) could be derived by comparing the expressions of $|\xi_i\rangle, |\zeta_j\rangle$ in Eqs. (31,38). That these vectors diagonalize the associated $\Gamma_{xy}$ is proven in the following theorem.

While realized in the basis (46), the expression (44) of $\Gamma_{xy}$ gets diagonalized by the same basis vectors – the diagonalization works because the vectors under consideration are orthonormal. Formally speaking,

**Theorem 5.** For $\Gamma_{xy}$ described in Eq. (44) but for equal error rates and realized in the basis (46),

$$\Gamma_{xy}|E_0\rangle = \gamma_0|E_0\rangle,$$

where $\gamma_0 = \sqrt{D(1 - D)(1 - D)} = \frac{1}{2}(\mathcal{G}^2 - \mathcal{G}^2)(1 - D)$ for equal error rates.

**Proof.** For equal error rates, Eq. (44) becomes

$$\Gamma_{xy} = \frac{1}{2}(\mathcal{G}^2 - \mathcal{G}^2)(1 - D)|E_0\rangle + D (|E_{22} - E_{33}|).$$

If we realize this expression in the basis (46), then

$$\Gamma_{xy}|E_0\rangle = \frac{1}{2}(\mathcal{G}^2 - \mathcal{G}^2)(1 - D)|E_0\rangle = \gamma_0|E_0\rangle,$$

so far $\{|E_{\lambda}\rangle\}$ are orthonormal, which indeed is true for Eq. (46). This completes the proof for $\lambda = 0$.

**Remark 6.** One can calculate and check that the eigenvalues of $\Gamma_{xy}$ described in eigenbasis (46) match those as in Eq. (45) calculated for the generic form of optimal $|\xi_i\rangle, |\zeta_j\rangle$ described by Eq. (38) but for equal error rates.

Connecting interactions (38) to the known instances (27,31) helped develop the intuition for finding the family of optimal POVMs hidden behind interactions (38). Now we are in a position to pinpoint the bases for which $\Gamma_{xy}$ in Eq. (44) gets diagonalized.
D. Optimal POVM corresponding to an optimal interaction in its generic form

In Theorem 4, it was shown that a specific rotation of the canonical basis $\{|E_\lambda\rangle\}$ yields an eigenbasis $\{|E_\lambda\rangle\}$ of $\Gamma_{xy}$ that corresponds to the optimal interaction (38). Now, we will show that not only the above specific rotation, but any rotation represented by an orthogonal linear transformation of the canonical basis $\{|E_\lambda\rangle\}$ yields an eigenbasis of $\Gamma_{xy}$ in Eq. (44).

Given an interaction, an optimal POVM corresponds to an orthonormal basis $\{|E_\lambda\rangle\}$ that diagonalizes $\Gamma_{xy}$ associated with that interaction. For interactions (38), the associated $\Gamma_{xy}$ is given by Eq. (44). Our task is to identify the bases, each of which diagonalizes the corresponding $\Gamma_{xy}$ realized in the same basis. First we observe that, for a set $\{|E_\lambda\rangle\}$ of vectors, and for projectors $\Gamma_{ii}$ in Eq. (44),

$$\Gamma_{ii}|E_\lambda\rangle = \gamma_\lambda |E_\lambda\rangle, \forall \lambda,$$

if and only if the vectors $|E_\lambda\rangle$ are orthonormal. In such case, it is guaranteed that the $\Gamma_{xy}$ in Eq. (44) gets diagonalized by the basis $\{|E_\lambda\rangle\}$, because

$$\Gamma_{xy}|E_\lambda\rangle = \gamma_\lambda |E_\lambda\rangle, \forall \lambda,$$

where the values of $\gamma_\lambda$ coincides with those in Eq. (45).

Since any rotation $R$ of the canonical basis $\{|E_\lambda\rangle\}$ produces an orthonormal basis, it diagonalizes the $\Gamma_{xy}$ of Eq. (44) realized in the same rotated basis. Hence, each of these rotated bases constitutes the optimal POVM for an interaction (38) realized in the same rotated basis.

To express the above idea mathematically, we introduce the notations below:

$$e := (|E_0\rangle, |E_1\rangle, |E_2\rangle, |E_3\rangle)^T, \quad \varepsilon := (|E_0\rangle, |E_1\rangle, |E_2\rangle, |E_3\rangle)^T,$$

and state the following result.

**Theorem 6.** Any orthogonal rotation $R$ of the canonical basis $\{|E_\lambda\rangle\}$, which is realized by

$$e = R\varepsilon,$$  \hspace{1cm} (47)

works as an orthonormal eigenbasis of $\Gamma_{xy}$ in Eq. (44) while the optimal interaction (38) is realized in the same rotated basis. To be precise, the rotated basis diagonalizes $\Gamma_{xy}$ in this case.

Note that in Eq. (47), orthonormality of the eigenbasis is preserved only when $R$ is an orthogonal matrix, and not any arbitrary linear transformation. Thus, for any orthogonal rotation $R$, the orthonormal basis $\{|E_\lambda\rangle\}$ realized by Eq. (47) corresponds to an optimal POVM while the optimal interaction (38) is also realized in the same rotated basis. To see how these optimal POVMs help Eq. (38) to generate the family of optimal interactions, we let the coefficient matrix of Eq. (38) as $D$. Then, an optimal POVM due to $e = R\varepsilon$ leads to an instantiation $De = DR\varepsilon$ of the optimal interaction. Thus, Eqs. (38) and (47) establishes a one-to-one correspondence between an optimal interaction $DR\varepsilon$ and the optimal POVM realizing $R\varepsilon$. Fixing a rotation $R$ provides an instance of such pairs $(DR\varepsilon, R\varepsilon)$. Here we create a subclass of such orthogonal rotation.

**Example 1.** Consider a canonical basis $\{|E_\lambda\rangle\}$ for Eve as given in Eq. (23). Let

$$|E_0\rangle = \sqrt{a}|E_0\rangle - \sqrt{1-a}|E_1\rangle, \quad |E_1\rangle = \sqrt{1-a}|E_0\rangle + \sqrt{a}|E_1\rangle, \quad |E_2\rangle = \sqrt{a}|E_2\rangle - \sqrt{1-a}|E_3\rangle, \quad |E_3\rangle = \sqrt{1-a}|E_2\rangle + \sqrt{a}|E_3\rangle.$$  \hspace{1cm} (48)

Since the coefficient matrix is orthogonal, $\{|E_\lambda\rangle\}_{\lambda \in \{0,1,2,3\}}$ forms an orthonormal eigenbasis for $\Gamma_{xy}$.

E. Achieving both optimal information gain (G) and optimal mutual information (I)

Identification of the optimal POVMs helped to unfold the family of optimal interactions that was hiding behind the unique expression (38). Equations (38) and (47), when considered together, provides a family of interaction-POVM pairs $(DR\varepsilon, R\varepsilon)$. Such a pair along with their counterpart in $u-v$ basis, by virtue of our construction of optimal interactions (38), should lead to optimal information gain by achieving the bounds in Eqs. (9,10), which in turn lead to optimal mutual information by achieving the bounds in Eqs. (12,13). However, for completeness, we show that such a pair satisfies the necessary and sufficient conditions given by Proposition 3 and therefore leads to optimality. Following this process, as an indicator for optimality, we establish in Lemma 4 an additional result regarding the sign of $\gamma_\lambda$.

Proof of the following theorem works on the unique expression $De$ of optimal interaction vectors rather than working on its representative pairs $(DR\varepsilon, R\varepsilon)$. The initial task is to find an expression for $|\xi_u\rangle, |\xi_v\rangle, |\zeta_u\rangle, |\zeta_v\rangle$ corresponding to Eq. (38). For this, we use Eqs. (42,43) in Eqs. (21,22), to derive the following intermediate result.

**Lemma 3.** For achieving the optimal information gain, we must have

$$|\xi_u\rangle = \sqrt{1 - D_{xy}} |\tilde{E}_0\rangle + \sqrt{D_{xy}} |\tilde{E}_2\rangle,$$

$$|\xi_v\rangle = \sqrt{1 - D_{xy}} |\tilde{E}_0\rangle - \sqrt{D_{xy}} |\tilde{E}_2\rangle,$$

$$|\zeta_u\rangle = \sqrt{1 - D_{xy}} |\tilde{E}_1\rangle - \sqrt{D_{xy}} |\tilde{E}_3\rangle,$$

$$|\zeta_v\rangle = \sqrt{1 - D_{xy}} |\tilde{E}_1\rangle + \sqrt{D_{xy}} |\tilde{E}_3\rangle.$$  \hspace{1cm} (49)

where the basis $\{|\tilde{E}_\lambda\rangle\}$ is as described in Eq. (43).

**Remark 7.** To get expressions of $|\xi_\lambda\rangle, |\zeta_\lambda\rangle$ in $u-v$ basis symmetric to those in $x-y$ basis, e.g., like [2, Eq. (52)], one must consider the canonical basis in the order $|E_\lambda\rangle = |x\rangle|x\rangle, |E_1\rangle = |y\rangle|y\rangle, |E_2\rangle = |x\rangle|y\rangle, |E_3\rangle = |y\rangle|x\rangle$, compatible with [2].
Theorem 7. The interaction given by Eqs. (38, 18) and a POVM corresponding to the eigenbasis given by Eq. (47) satisfy the necessary and sufficient conditions given by Proposition 3 and therefore attain optimal information gain and optimal mutual information.

Proof. From Eq. (17), we have

\[ |U_{\lambda u} \rangle = B_u \otimes \sqrt{E_\lambda} |U \rangle = B_u \otimes E_\lambda |U \rangle \]

\[ = \sqrt{1 - D_{uv}} \langle B_u |u \rangle \otimes (E_\lambda |\xi_u \rangle) \]

\[ + \sqrt{D_{uv}} \langle B_u |v \rangle \otimes (E_\lambda |\zeta_v \rangle) , \]

by Eq. (20).

Since \( B_u |u \rangle = |u \rangle, B_u |v \rangle = 0 \), and \( E_\lambda |\xi_u \rangle = \langle E_\lambda |\xi_u \rangle |E_\lambda \rangle \), we get,

\[ |U_{\lambda u} \rangle = \sqrt{1 - D_{uv}} \langle E_\lambda |\xi_u \rangle |u \rangle |E_\lambda \rangle . \]

Similarly,

\[ |V_{\lambda u} \rangle = \sqrt{D_{uv}} \langle E_\lambda |\zeta_v \rangle |u \rangle |E_\lambda \rangle . \]

Here, we want equality in magnitude between \( \langle E_\lambda |\xi_u \rangle \) and \( \langle E_\lambda |\zeta_v \rangle \). Now, by Eq. (49), \( \langle E_\lambda |\zeta_v \rangle \) takes values

\[ \frac{1}{\sqrt{2}} \sqrt{1 - D_{xy}}, \frac{1}{\sqrt{2}} \sqrt{1 - D_{xy}}, \frac{1}{\sqrt{2}} \sqrt{D_{xy}}, \frac{1}{\sqrt{2}} \sqrt{D_{xy}} ; \]

whereas, \( \langle E_\lambda |\xi_u \rangle \) takes values

\[ \frac{1}{\sqrt{2}} \sqrt{1 - D_{xy}}, - \frac{1}{\sqrt{2}} \sqrt{1 - D_{xy}}, \frac{1}{\sqrt{2}} \sqrt{D_{xy}}, - \frac{1}{\sqrt{2}} \sqrt{D_{xy}} , \]

respectively for \( \lambda = 0, 1, 2, 3 \). Therefore,

\[ |V_{\lambda u} \rangle = \varepsilon_\lambda \sqrt{D_{uv}} |U_{\lambda u} \rangle , \]

where,

\[ \varepsilon_0 = +1, \quad \varepsilon_1 = -1, \quad \varepsilon_2 = +1, \quad \varepsilon_3 = -1 . \] (50)

Similarly, one may calculate to verify that

\[ |U_{\lambda v} \rangle = \varepsilon_\lambda \sqrt{\frac{D_{uv}}{1 - D_{uv}}} |V_{\lambda u} \rangle , \]

for the same combination of \( \varepsilon_\lambda \) as in Eq. 50. This completes the proof of the theorem.

Further, we take the opportunity to establish a direct relation between the sign parameter \( \varepsilon_\lambda \) and the signs of eigenvalues \( \gamma_\lambda \).

Lemma 4. For optimal \( G \),

\[ \varepsilon_\lambda = \text{sgn} \gamma_\lambda . \] (51)

Proof. For optimal \( G \), \( \Gamma \) is a diagonal matrix with diagonal entries \( \gamma_\lambda \). Thus, for signals sent in \( x-y \) basis,

\[ \gamma_\lambda = \text{tr}(\Gamma_{xy} E_\lambda) = \frac{1}{2} [\text{tr}(\rho_x E_\lambda) - \text{tr}(\rho_y E_\lambda)] = \frac{1}{2}(P_{\lambda x} - P_{\lambda y}) . \]

By Eq. (16),

\[ \varepsilon_\lambda = \text{sgn} (Q_{x\lambda} - Q_{y\lambda}) = \text{sgn} (P_{\lambda x} - P_{\lambda y}) = \text{sgn} \gamma_\lambda , \]

which establishes the relation.

Remark 8. By Lemma 4, another indication for optimality is that Eq. (50) should match with the signs of the eigenvalues \( \gamma_\lambda \) of \( \Gamma_{xy} \) as in Eq. (45), which indeed happens here. Therefore, for any rotation of the canonical basis, a pair \( (\text{DR}_X, \text{R}_Z) \) of optimal interaction and corresponding optimal POVM in Eqs. (38, 47) achieves optimality.

Here we summarize the results achieved so far. While Eq. (38) captures a class of optimal interactions in a unique form, Eq. (47) depicts the class of optimal POVMs for those interactions. Combining Eqs. (38, 47) we get the whole class of optimal interactions expressed in canonical basis. Fixing a rotation matrix \( \text{R} \) then produces a particular instance of an optimal interaction,
while varying $\mathbf{R}$ produces the whole class of optimal interactions. Although there are infinitely many optimal interactions while expressed in canonical basis, they all have a unique form \( (38) \) while written in eigenbasis of $\Gamma_{xy}$. Figure 1 illustrates this fact. Each round node in the figure denotes that the two input results together derive the output result.

V. A DISCUSSION ON CONNECTION BETWEEN OUR RESULTS AND THOSE OF FUCHS ET AL. [2]

Here we show that the instances of an optimal interaction presented in \cite{2} is a special case of the generalized unique form of the optimal interaction that we have derived. Moreover, we generate a new instance (different from the two instances of \cite{2}) of the optimal interaction to add more clarity to our achievement.

As discussed earlier, Eqs. \((38)\) and \((47)\) are key ingredients to generate different instances of the pair \((\mathbf{D}\mathbf{R}x, \mathbf{R}e)\) of optimal interaction and corresponding optimal POVM by varying rotation $\mathbf{R}$ of the canonical basis. For a special type of the orthogonal matrix $\mathbf{R}$ as given by Example 1, we combine these results and write an optimal interaction in terms of the canonical basis as below:

\[
\begin{align*}
|\xi_x\rangle &= (\mathcal{D}_{uv}\sqrt{a} + \mathcal{D}_{uv}\sqrt{1-a}) |\xi_0\rangle, \\
+ (\mathcal{D}_{uv}\sqrt{a} - \mathcal{D}_{uv}\sqrt{1-a}) |\xi_1\rangle, \\
|\xi_y\rangle &= (\mathcal{D}_{uv}\sqrt{a} + \mathcal{D}_{uv}\sqrt{1-a}) |\xi_0\rangle, \\
+ (\mathcal{D}_{uv}\sqrt{a} - \mathcal{D}_{uv}\sqrt{1-a}) |\xi_1\rangle, \\
|\xi_z\rangle &= (\mathcal{D}_{uv}\sqrt{a} + \mathcal{D}_{uv}\sqrt{1-a}) |\xi_2\rangle, \\
+ (\mathcal{D}_{uv}\sqrt{a} - \mathcal{D}_{uv}\sqrt{1-a}) |\xi_3\rangle, \\
|\xi_y\rangle &= (\mathcal{D}_{uv}\sqrt{a} + \mathcal{D}_{uv}\sqrt{1-a}) |\xi_2\rangle, \\
+ (\mathcal{D}_{uv}\sqrt{a} - \mathcal{D}_{uv}\sqrt{1-a}) |\xi_3\rangle. \\
\end{align*}
\]

For unequal error rates, Eq. \((27)\) is a special case (apart from a permutation of the canonical basis) with $a = 1$ in Eq. \((52)\). Similarly, for equal error rates ($D_{xy} = D_{uv} = D$), Eq. \((31)\) is a special case with $a = \mathcal{D}^2$ in Eq. \((52)\). One may consider innumerable such optimal interactions (and corresponding optimal POVMs) by tuning the rotation parameter $a$ in the range $[0, 1]$. One such example is given below for unequal error rates.

**Example 2.** Let $a = \frac{1}{2}$. Thus the optimal interaction in Eq. \((52)\) becomes

\[
\begin{align*}
|\xi_x\rangle &= \sqrt{1 - D_{uv}} |\xi_0\rangle - \sqrt{D_{uv}} |\xi_1\rangle, \\
|\xi_y\rangle &= \sqrt{1 - D_{uv}} |\xi_0\rangle + \sqrt{D_{uv}} |\xi_1\rangle, \\
|\xi_z\rangle &= \sqrt{1 - D_{uv}} |\xi_2\rangle - \sqrt{D_{uv}} |\xi_3\rangle, \\
|\xi_y\rangle &= \sqrt{1 - D_{uv}} |\xi_2\rangle + \sqrt{D_{uv}} |\xi_3\rangle. \\
\end{align*}
\]
FIG. 2: Optimal interaction: unique expression to specific instantiations

![Diagram](image)

and the corresponding optimal POVM is captured by

\[
\begin{align*}
|E_0\rangle &= \frac{1}{\sqrt{2}} (|E_0\rangle - |E_1\rangle), \\
|E_1\rangle &= \frac{1}{\sqrt{2}} (|E_0\rangle + |E_1\rangle), \\
|E_2\rangle &= \frac{1}{\sqrt{2}} (|E_2\rangle - |E_3\rangle), \\
|E_3\rangle &= \frac{1}{\sqrt{2}} (|E_2\rangle + |E_3\rangle).
\end{align*}
\]

(54)

One may easily check that the interaction presented here is indeed optimal. Clearly, the general form of the optimal interaction provided in this paper yields different choices of those in [2]. Moreover, it’s implementation is independent of equal or unequal error rates.

At this stage, we weigh the results achieved by us. Fuchs et al. [2] came up with two different configurations for optimal interactions expressed in canonical basis. For the first configuration (Eq. 25), they described the corresponding POVM (Eq. 26) w.r.t. the canonical basis, while for their second configuration (Eq. 31), we have deduced the corresponding POVM (Eq. 46) in terms of the canonical basis. We have presented one more instance of an optimal interaction (Eq. 53) and the corresponding POVM (Eq. 54) w.r.t. the canonical basis. Table II describes the general form of the optimal interaction and also shows its four specific instantiations, of which the first two coincide with those of Fuchs et al. [2] and the later two with our examples discussed earlier, the corresponding POVMs are also captured there.

For each of these three instances of the optimal interaction, one may use the relation between the eigenbasis and the canonical basis (looking at the POVM) to express the interaction w.r.t. the eigenbasis and notice that the final form becomes the same (Eq. 38) for all these cases. It turns out that every possible instances of an optimal interaction written w.r.t. the canonical basis can be transformed to a unique description (Eq. 38) in terms of the eigenbasis via the corresponding POVM. This is the significance of our work. We could establish that there exists infinitely many possible instances of an optimal interaction represented in a canonical basis, but they all have a unique representation while expressed in the eigenbasis. Feeding an optimal POVM to the unique form of the optimal interaction produces a specific instance of an optimal interaction. This is depicted in Figure 2. Since an optimal interaction has an unique form and the form in Fuchs et al. [2] is a special case, any instance of such an optimal interaction will achieve the same optimal information gain $G^*$ benchmarked in [2], neither more nor less.

VI. CONCLUSION

For the BB84 quantum key distribution protocol, we have established a unique form describing the optimal interaction followed by the class of corresponding optimal measurements for the optimal information gain an eavesdropper can obtain for a given average disturbance when her interaction and measurements are performed signal by signal. We have shown that the choice of optimal interaction in [2], for equal as well as unequal error rates, is a special case of the form provided by us.

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