Loss-tolerant quantum cryptography with imperfect sources

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Introduction.— Quantum key distribution (QKD) [1] allows two distant parties, Alice and Bob, to distribute a secret key, which is essential to achieve provable secure communications [2]. The field of QKD has progressed very rapidly over the last years, and it now offers practical systems that can operate in realistic environments [3, 4].

In principle, quantum key distribution (QKD) offers unconditional security based on the laws of physics. In practice, flaws in the state preparation undermine the security of QKD systems, as standard theoretical approaches to deal with state preparation flaws are not loss-tolerant. An eavesdropper can enhance and exploit such imperfections through quantum channel loss, thus dramatically lowering the key generation rate. Crucially, the security analyses of most existing QKD experiments are rather unrealistic as they typically neglect this effect. Here, we propose a novel and general approach that makes QKD loss-tolerant to state preparation flaws. Importantly, it suggests that the state preparation process in QKD can be significantly less precise than initially thought. Our method can widely apply to other quantum cryptographic protocols.

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Our work builds on the security proof introduced by Koashi [12] based on complementarity of conjugate observables, X and Z. Also, it employs the idea of "rejected data analysis" [13], i.e., we consider data obtained when Alice’s and Bob’s measurement bases are different, as well as the fact that any qubit state can be written in terms of Pauli matrices. Therefore, to calculate the objective quantity, i.e., the so-called phase error rate, it is enough to find the transmission rates of these matrices.

In so doing, we can: (i) dramatically improve the key rate and achievable distance of QKD with modulation errors (see Fig. 1 for details); (ii) show that the three-state scheme [16, 17] gives precisely the same key rate as the BB84 protocol [18]. This result is outstanding, as it implies that one of the signals sent in BB84 is actually redundant [19]. In addition, our technique is: (iii) applicable to measurement-device-independent QKD (mdiQKD) [20]; (iv) applicable to other QKD schemes including the six-state protocol [21]. It can be shown, for instance, that a particular four-state scheme can post-process its data following the specifications of the six-state protocol [21]. That is, it can use the correlation between phase and bit errors to increase its key rate. (v) Our method also applies to other quantum cryptographic applications (e.g., bit commitment based on the noisy storage model [22]).

To simplify the discussion, we assume collective attacks, i.e., Eve applies the same quantum operation to each signal. However, our results also hold against coherent attacks by just applying either the quantum De Finetti theorem [23] or Azuma’s inequality [24–26] (see Appendix A for details). Moreover, for simplicity, we consider the asymptotic scenario where Alice sends Bob an infinite number of signals. In addition, we assume to enhance the imperfections through channel loss.

Appendix A for details). Moreover, for simplicity, we consider the asymptotic scenario where Alice sends Bob an infinite number of signals. In addition, we assume
that there is no side-channel in the source. That is, we consider that the single-photon components of Alice’s signals are qubits, and we analyze an important type of state preparation flaws, namely modulation errors due to slightly over or under modulation of the signal’s phase/polarization by an imperfect apparatus. Also, we assume that Bob’s measurement device satisfies two conditions: random basis choice and basis-independent detection efficiency. The former is fulfilled if Bob selects at random between two or more measurement settings; one for key distillation and the others for parameter estimation. The latter is satisfied if the probability of having a detection event is independent of Bob’s measurement setting choice. With mdiQKD, we can waive these two conditions and allow the detection system to be untrusted.

Prepare & measure three-state protocol. In this scheme [16, 17], Alice sends Bob three pure states, \(|\phi_{0x}\rangle = |0_x\rangle, |\phi_{1x}\rangle = |1_x\rangle\) and \(|\phi_{0z}\rangle = |0_z\rangle\), which she selects independently at random for each signal. Here, the states \(|j_x\rangle = |0_x\rangle + (-1)^j|1_x\rangle|/\sqrt{2}\), with \(j \in \{0, 1\}\). On Bob’s side, he measures the signals received using either the X or the Z basis, which he selects as well independently at random for each incoming signal. After that, Alice and Bob announce their basis choices, and they estimate the bit and phase error rate. We assume that they generate a secret key only from those instances where both of them select say the Z basis.

In the following, we present a precise phase error rate estimation technique that uses the bases mismatch events information. The key idea is very simple yet potentially very useful: since any qubit state can be written in terms of Pauli matrices, it is enough to find the transmission rates of these operators; this will become clear below. First, we introduce some notation.

In particular, let \({\cal M}_{0\beta}, {\cal M}_1\beta, {\cal M}_\beta\) denote the elements of Bob’s positive-operator valued measure (POVM) associated with the basis \(\beta \in \{X, Z\}\). \(\hat{M}_\beta\) and \(\hat{M}_\beta\) correspond, respectively, to the bit values 0 and 1, and \(\hat{M}_\beta\) represents the inconclusive event. These operators do not necessarily act on a qubit space, i.e., Eve can send Bob any higher-dimensional state. The essential assumption here is that \(\hat{M}_\beta\) is the same for both bases [12]. Also, we denote as \(Y_{s\beta,j\alpha}\), with \(s, j \in \{0, 1\}\) and \(\beta, \alpha \in \{X, Z\}\), the joint probability that Alice prepares the state \(|\phi_{j\alpha}\rangle\) and Bob measures it in the \(\beta\) basis and obtains a bit value \(s\).

Theorem. The prepare & measure three-state protocol described above provides a secret key rate \(R \propto 1 - h(e_x) - h(e_z)\), where \(h(x) = -x \log_2 x - (1 - x) \log_2 (1 - x)\) is the binary Shannon entropy, \(e_x\) is the bit error rate, and \(e_z\) is the phase error rate given by

\[
e_x = \frac{Y_{0z,0x} + Y_{0z,1x} + Y_{1z,0x} - Y_{1z,1x}}{Y_{0z,0x} + Y_{0z,1x} + Y_{1z,0x} + Y_{1z,1x}}.
\]

Notably, \(e_x\) coincides with that of the BB84 protocol.

This result is remarkable because it implies that the three-state protocol can achieve precisely the same performance as the BB84 scheme, since both protocols can obtain the exact value for the phase error rate \(e_x\) together with the bit error rate \(e_z\). That is, the additional signal \(|1_x\rangle\) that is sent in BB84 seems to be unnecessary. This means, for instance, that in those implementations of the BB84 protocol that use four laser sources one could keep one laser just as back-up in case one of them fails, without any decrease in performance [27]. This also reduces the consumption of random numbers to select the different sources. Our security analysis differs from that provided in Ref. [17] in that it requires less privacy amplification (PA), and, consequently, it can deliver a higher secret key rate. Next, we present the proof for the Theorem.

Proof. The preparation of the Z-basis states \(|\phi_{0x}\rangle\) and \(|\phi_{1x}\rangle\) can be formulated in an entanglement based version of the protocol as follows. Alice first creates a source state \(|\Psi_Z\rangle_{AB} = (|0_x\rangle_A|0_x\rangle_B + |1_x\rangle_A|1_x\rangle_B)/\sqrt{2}\). Afterwards, she measures system A in the Z basis, thereby producing the correct signal state at site B that is sent to Bob. The phase error rate \(e_x\) is defined as the bit error rate that Alice and Bob would observe if they measure \(|\Psi_Z\rangle_{AB}\) in the X basis. Importantly, if \(N_z\) denotes the number of sifted bits in the Z basis, to distill a secure key Alice and Bob need to sacrifice \(N_z h(e_x)\) bits in the PA step.

To calculate \(e_x\), we define a virtual protocol where Alice and Bob measure \(|\Psi_Z\rangle_{AB}\) in the X basis. This state can be equivalently written as \(|\Psi_Z\rangle_{AB} = (|0_x\rangle_A|0_x\rangle_B + |1_x\rangle_A|1_x\rangle_B)/\sqrt{2}\). That is, if Alice measures system A in the X basis and obtains the bit value \(j \in \{0, 1\}\), she effectively prepares the signal \(|j_x\rangle_B\) at site B. This means that

\[
e_x = (Y_{0z,0x} + Y_{1z,0x})/(Y_{0z,0x} + Y_{0z,1x} + Y_{1z,0x} + Y_{1z,1x}).
\]

Importantly, the probabilities \(Y_{s\beta,j\alpha}\), with \(s \in \{0, 1\}\), are directly observed in the experiment because in the actual protocol Alice sends Bob the signal \(|0_x\rangle\).

To obtain the terms \(Y_{s\beta,j\alpha}\), we use the fact that any qubit state can be decomposed in terms of the identity and the three Pauli matrices. For this, we first rewrite

\[
Y_{s\beta,j\alpha} = \frac{1}{6} \text{Tr}[\hat{D}_{s\beta}(P_{\{1\beta\}})],
\]

where \(P_{\{\beta\}} = \langle \beta | \langle \beta \rangle\), \(\hat{D}_{s\beta} = \sum_k \hat{A}_k M_{s\beta} A_k\) with \(A_k\) being an arbitrary operator (see Appendix A), and 1/6 is the probability that Alice emits \(|1_x\rangle\) and Bob chooses the X basis. Then, we define \(q_{s\alpha|x}\) as

\[
q_{s\alpha|x} = \text{Tr}[\hat{D}_{s\beta}(\sigma_{\beta j\alpha})]/2 \propto \hat{\sigma}_{\beta j\alpha}/2, \text{ where } \hat{\sigma}_{\beta j\alpha}, \text{ with } t \in \{\text{Id, } x, z\},
\]

denotes, respectively, the identity and two of the Pauli operators. With this notation, and using \(P_{\{1\beta\}} = (\text{Id} - \hat{\sigma}_{\beta 0\beta})/2\), we have that \(Y_{s\beta,j\alpha} = \frac{1}{6}(q_{s\alpha|x} - q_{s\alpha|z})\).

Finally, to calculate \(q_{s\alpha|x} \propto |s\alpha|\) we use the following constraints,

\[
Y_{s\alpha,0s} = \frac{1}{6} \text{Tr} [\hat{D}_{s\beta}(P_{\{00\beta\}})] = \frac{1}{6}(q_{s\alpha|x} + q_{s\alpha|z}),
\]

\[
Y_{s\alpha,1s} = \frac{1}{6} \text{Tr} [\hat{D}_{s\beta}(P_{\{10\beta\}})] = \frac{1}{6}(q_{s\alpha|x} - q_{s\alpha|z}),
\]

\[
Y_{s\alpha,0s} = \frac{1}{6} \text{Tr} [\hat{D}_{s\beta}(P_{\{01\beta\}})] = \frac{1}{6}(q_{s\alpha|x} + q_{s\alpha|z}).
\]

Recall that the probabilities \(Y_{s\beta,j\alpha}\) are independent, since the vectors \(\vec{V}_{j\alpha} := (p_{0\beta}^{j\alpha}, p_{1\beta}^{j\alpha}, p_{z\beta}^{j\alpha})\), with \(p_{\beta}^{j\alpha}\) being the \(w = x, y, z\) component of the Bloch vector of the state \(|\phi_{j\alpha}\rangle\), are mutually linearly independent. Thus, by solving Eqs. (2)-(4)
one can obtain the exact value for $q_{s(i)}$; we find that
\[ Y_{s,i} = Y_{s,0i} + Y_{s,1i} - Y_{s,0s} \]
Substituting this expression into the definition of $e_x$, we obtain Eq. (1).

So far, for simplicity, we have considered that Alice sends Bob single-photon states. However, our results can be used as well when she prepares phase-randomized weak coherent pulses (WCPs) in combination with decoy states \[28\]. This is so because the decoy-state method allows Alice and Bob to estimate the relevant probabilities $Y_{s,0i}$, $Y_{s,1i}$, and $Y_{s,0s}$ associated with the single-photon signals. In addition, the analysis above can be easily extended to include modulation errors (see Appendix B). This scenario is shown in the simulation.

*Simulation.*—Here we evaluate the performance of a three-state protocol based on WCPs together with decoy states in the presence of modulation errors. For simplicity, we consider the asymptotic situation where Alice uses an infinite number of decoy settings. Moreover, we assume that she employs phase-coding, as this is usually the preferential coding choice in optical fibre implementations. However, our analysis applies as well to other coding schemes, e.g., polarization and time-bin coding.

More precisely, we consider that Alice sends Bob signals of the form $|e^{i\xi} \sqrt{\alpha}\rangle |e^{i(\xi + \theta_\Lambda + \theta_3/\pi)} \sqrt{\alpha}\rangle_s$, where $\xi \in [0, 2\pi)$ is a random phase, $\theta_\Lambda \in \{0, \pi/2, \pi\}$ encodes Alice’s information, the term $\theta_3/\pi$ with $\delta \geq 0$ models an example of phase modulation errors, and $|e^{i\xi} \sqrt{\alpha}\rangle_s$ is a coherent state with mean photon number $\alpha$. The subscripts $r$ and $s$ are used to denote, respectively, the reference and signal mode. In this scenario, the single-photon components of Alice’s signals lie on a plane of the Bloch sphere. In addition, we assume the same phase modulation error on Bob’s side, i.e., his phase modulation is $\theta_3 + \theta_3/\pi$ when he chooses $\theta_3 \in \{0, \pi/2\}$. Importantly, since $\delta \geq 0$, Alice’s and Bob’s modulation errors do not cancel each other, but they only increase the total modulation error.

The resulting lower bound on the secret key rate $R$ for different values of the error parameter $\delta$ is shown in Fig. 1 (see Appendix C). For comparison, this figure includes as well a lower bound on $R$ for the asymptotic decoy-state BB84 protocol. For the latter, we use results from Ref. [14], which are based on the GLLP security analysis \[13\], and we use the same phase modulation model described above with $\theta_\Lambda \in \{0, \pi/2, \pi, 3\pi/2\}$. As shown in the figure, our phase error rate estimation technique can significantly outperform GLLP in the presence of modulation errors. In particular, while GLLP delivers a key rate that decreases rapidly when $\delta$ increases (since it considers the worst case scenario where losses can increase the fidelity flaw \[13\]), our method produces an almost constant key rate independently of $\delta$. The slight performance decrease of the three-state protocol when $\delta$ increases is due to the increase of the bit error rate $e_x$ stemming from imperfect phase modulations.

*Measurement-device-independent QKD.*—We consider a modified version of mdiQKD \[20\] where Alice and Bob send Charles the states $|\phi_0\rangle$, $|\phi_1\rangle$, and $|\phi_2\rangle$. Charles is supposed to perform a Bell state measurement that projects them into a Bell state, and then he announces his results. Alice and Bob keep the data associated with the successful results, post-select the events where they employ the same basis, and say Bob applies a bit flip to part of his data \[20\]. They use the Z basis (X basis) for key distillation (parameter estimation).

In the following, we apply the phase error rate estimation method introduced above to mdiQKD. Now, $e_x$ can be expressed as

\[ e_x = \frac{Y_{0^+0+1s} + Y_{0^-1s0s}}{Y_{0^+0+1s} + Y_{0^+1s0s} + Y_{0^-0+1s} + Y_{0^-1s0s}} \]

where $Y_{0^+jxs}$, with $j, k \in \{0, 1\}$, denotes the joint probability that Alice and Bob send Charles $|jx\rangle$ and $|ks\rangle$ respectively, and Charles declares the result $|\phi_t\rangle$ (although he might be dishonest). This probability can be
expressed as $Y_{\phi^+, j \cdot k_\alpha} = \frac{1}{9} \text{Tr}[\hat{D}_{\phi^+} \hat{P}(j_{\alpha}) \otimes \hat{P}(k_\alpha)]$ for a certain operator $\hat{D}_{\phi^+}$. Now, we follow the technique described previously. We define $q_{\phi^+, |x\rangle} = \text{Tr}(\hat{D}_{\phi^+} \hat{\sigma}_x \otimes \hat{\sigma}_x)/4$ with $s, t \in \{\text{Id}, x, z\}$, and we use $\hat{P}(j_{\alpha}) = [\hat{1} + (-1)^{j_{\alpha}/2} \hat{\sigma}_x]/2$ to write $Y_{\phi^+, j \cdot k_\alpha}$ in terms of $q_{\phi^+, |\text{Id}, \text{Id}\rangle}$, $q_{\phi^+, |x, \text{Id}\rangle}$, $q_{\phi^+, |\text{Id}, x\rangle}$, and $q_{\phi^+, |x, x\rangle}$. Finally, to calculate these coefficients we solve the following set of linear equations,

$$Y_{\phi^+, j \cdot k_\alpha} = \frac{1}{9} \text{Tr}\left[\hat{D}_{\phi^+} \hat{P}(j_{\alpha}) \otimes \hat{P}(k_\alpha)\right],$$

$$Y_{\phi^+, 0_{\alpha} k_\alpha} = \frac{1}{9} \text{Tr}\left[\hat{D}_{\phi^+} \hat{P}(0_{\alpha}) \otimes \hat{P}(k_\alpha)\right],$$

$$Y_{\phi^+, j \cdot 0_{\alpha}} = \frac{1}{9} \text{Tr}\left[\hat{D}_{\phi^+} \hat{P}(0_{j}) \otimes \hat{P}(\phi_{k_\alpha})\right],$$

$$Y_{\phi^+, 0_{\alpha} 0_{\alpha}} = \frac{1}{9} \text{Tr}\left[\hat{D}_{\phi^+} \hat{P}(\phi_{0_{\alpha}}) \otimes \hat{P}(\phi_{0_{\alpha}})\right].$$

For simplicity, here we have omitted the explicit dependence of Eqs. (6-9) with $q_{\phi^+, |x\rangle}$, and $\frac{\pi}{4} (0 < \gamma < 1)$ is the probability that Alice and Bob send Charles $|\phi_{j_{\alpha}}\rangle$ and $|\psi_{k_\alpha}\rangle$ respectively, and they sacrifice such instances as test bits. Unlike the three-state protocol introduced above, note that now we need such test bits from the sifted bits in the Z basis to estimate $\varepsilon_x$. Importantly, since the set of vectors $\mathcal{V}_{j_{\alpha}}$ associated with the states $\hat{P}(|\phi_{j_{\alpha}}\rangle)$ are mutually linearly independent, Eqs. (6-9) are also independent. Therefore, one can obtain the exact value for all $q_{\phi^+, |x\rangle}$, and, consequently, also for $Y_{\phi^+, j \cdot k_\alpha}$ and $\varepsilon_x$.

Like the three-state protocol, the mdiQKD scheme above is also loss-tolerant to modulation errors. That is, by combining our work with mdiQKD, we can simultaneously address flaws in state preparation and detection systems and obtain a high secret key rate.

**Discussion.**— To find the phase error rate in a QKD protocol one has to estimate the transmission rate of certain states, which might not have been in the actual scheme (e.g., the signal $|1_x\rangle$ in the three-state protocol), based on the observed data. As any qubit state can be written in terms of the identity and Pauli matrices, it is enough to find the transmission rates of these operators. In the three-state scheme, the states $|\phi_{0_{\alpha}}\rangle$ and $|\phi_{1_{\alpha}}\rangle$ give the transmission rate of $\hat{1}$ and $\hat{\sigma}_x$. Thus, by sending any other state on the X-Z plane of the Bloch sphere (e.g., the signal $|0_x\rangle$), one can determine the transmission rate of $\hat{\sigma}_x$ and, consequently, of any qubit state in that plane, including $|1_x\rangle$. In general, we have that as long as the terminal points of the Bloch vectors of the three states form a triangle it is always possible to estimate $\varepsilon_x$ precisely (see Appendix A).

Similarly, if Alice sends Bob four different qubit states, whose vectors $\mathcal{V}_{j_{\alpha}}$ are mutually linearly independent, i.e., the terminal points of their Bloch vectors form a triangular pyramid, one can obtain the transmission rate of any Pauli operator, including the identity matrix, and, therefore, also the exact transmission rate of any qubit state (see Appendix A). In the original mdiQKD scheme [20] this implies, for instance, that Alice and Bob could determine the bit error rate associated to the virtual state that they would generate when measuring the first subsystem of $|\psi_Z\rangle = (|0_x\rangle|\phi_{0_{\alpha}}\rangle + |1_x\rangle|\phi_{1_{\alpha}}\rangle)/\sqrt{2}$ in the Y-basis. Here $C$ denotes the system that is sent to Charles. As a result, they could directly use this information to improve the achievable secret key rate. In standard prepare-and-measure QKD protocols, however, the estimation of the fictitious Y-basis error rate requires that Bob performs a measurement in that basis (see Appendix A). In addition, the basis-independent detection efficiency assumption must hold and Bob’s POVM elements must act on a qubit space. This is so because in order to exploit the correlation Alice and Bob need to share qubit states. Note, however, that this last requirement could be avoided by using either the universal squash idea or the detector-decoy method. That is, by including an additional phase modulator on Bob’s side (to perform the Y-basis measurement) one could enhance the performance of several practical systems that generate such four states, e.g., those based on the BB84 protocol or on the coherent-one-way (COW) scheme.

We have discussed the phase error rate estimation problem, which affects the PA step of a QKD protocol. To generate a secure key, however, it is also important that the bit error rate, which affects the error-correction step, is small enough. In this respect, our analysis suggests that while it is important to have a precise state preparation in the key generation basis, that of the other basis is not as essential, which simplifies experimental implementations. For instance, with our results, mdiQKD only needs to align one basis well and can tolerate substantial errors in the alignment of the other bases.

Finally, we would like to emphasize that our technique requires a complete characterization of the signal states transmitted. In practice, however, it might be easier to estimate a set of states that very likely contains the signals prepared. In this case, one could directly apply our method by just selecting the signal from that set that minimizes the key rate. Importantly, our results show that the effect of modulation errors on the performance of practical QKD systems is almost negligible.

**Conclusion.**— We have introduced a phase error rate estimation method that makes QKD loss-tolerant to state preparation flaws. It uses information from bases mismatch events. We have applied this technique to different practical QKD systems and we have shown that it can substantially improve their key generation rate and covered distance when compared to the standard GLLP result. Our work constitutes an important step towards secure QKD with imperfect devices.

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Appendix A: Three-state protocol & coherent attacks

Here we present the security proof for the three-state protocol. We consider that Alice and Bob distill key only from those events where both of them use the Z basis, while the events where Bob employs the X basis are used for parameter estimation.

As already introduced in the main text, the preparation of the Z-basis states can be equivalently described as follows. Alice first generates a signal state $|\psi_i\rangle_{AB}$ for parameter estimation.

Next, we calculate these conditional probabilities. For this, let $|\hat{\Phi}_{sh,B}\rangle = |\psi_{l-1}\rangle_{sh,B}|\varphi_{l}\rangle_{sh,B}|\varphi_{r}\rangle_{sh,B}$ denote the state prepared by Alice in an execution of the protocol. Here, $|\varphi_{l-1}\rangle_{sh,B}$, $|\varphi_{l}\rangle_{sh,B}$, and $|\varphi_{r}\rangle_{sh,B}$ represent, respectively, Alice’s signals in the first $l-1$ runs, in the $l$th run, and in the rest of runs.

This state evolves according to Eve’s unitary transformation, $\hat{V}_{BE}$, on Bob’s system B and on her system E as follows,

$$\hat{V}_{BE}|\hat{\Phi}_{sh,B}\rangle_{BE} = \sum_{k} \hat{B}_{k,B}|\hat{\Phi}_{sh,B}\rangle_{BE}|k\rangle_{E},$$

(A2)

where $\hat{B}_{k,B}$ is a Kraus operator acting on system B. Importantly, $\hat{V}_{BE}$ and $\hat{B}_{k,B}$ are independent of the state preparation process. This is so because the classical communication between Alice and Bob is done after finishing the measurements. Let the joint operator

$$\hat{O}_{l-1,sh,B} = \otimes_{u=1}^{l-1} \hat{M}_{sh,\varphi_{u}},$$

(A3)

where $\hat{M}_{sh,\varphi_{u}}$ denotes the Kraus operator associated to the $u^{th}$ measurement outcome of the shield system $sh$ and Bob’s $u^{th}$ measurement outcome. The joint state in the $l^{th}$ run of the protocol, $|\psi_{l}\rangle_{AB}$, conditioned on the measurement outcomes $O_{l-1}$ of the first $l-1$ joint

$$\psi_{l}\rangle_{AB} = |\varphi_{l}\rangle_{sh,B}|\varphi_{r}\rangle_{sh,B},$$

(A1)
systems can then be written as

\[ \rho_{I|O_{l-1}}^{sh,B} = \frac{\rho_{I|O_{l-1}}^{sh,B}}{p(l)}, \]

\[ \delta_{I|O_{l-1}}^{sh,B} := \sum_k \text{Tr} \left[ \hat{P} \left( \hat{O}_{l-1,sh,B} \hat{B}_{k,B} | \Phi \right)_{sh,B} \right], \]

\[ p(l) := \text{Tr} \left( \delta_{I|O_{l-1}}^{sh,B} \right), \]

where \( \text{Tr} \) represents the partial trace over all systems except the \( l \)th sh and B systems. Equivalently, \( \delta_{I|O_{l-1}}^{sh,B} \) can be rewritten as

\[ \delta_{I|O_{l-1}}^{sh,B} = \sum_k \sum_{\tilde{x}_{l-1,\tilde{x}_r}} \hat{P} \left( \hat{A}_{k,B}^{(\tilde{x}_{l-1},\tilde{x}_r)} | \varphi \right)_{sh,B}, \]

\[ \text{where} \quad \hat{A}_{k,B}^{(\tilde{x}_{l-1},\tilde{x}_r)} := \langle \tilde{x}_r | (\tilde{x}_{l-1},| \hat{O}_{l-1,sh,B} \hat{B}_{k,B} | \varphi \rangle_{sh,B}. \]

Here \( \{ \langle \tilde{x}_r | \right\} \{ \langle \tilde{x}_{l-1} | \} \) is bases for all the remaining systems after the \( l \)th run (for the first \( l-1 \) joint systems). Importantly, Eq. (A5) states that the \( l \)th joint system is subjected to Eve’s action and her action depends on all the previous measurement outcomes on the first \( l-1 \) joint systems.

Now, to determine the probability distribution for the different paths in Fig. 2, we measure the shield system sh using the basis \( \{ |c \rangle \} \) and Bob’s system using the X basis. The probability of obtaining \( c \) and the bit value \( s_x \) conditioned on \( O_{l-1} \) is given by

\[ Y_{s_x,c|O_{l-1}} = \frac{P(c)}{p(l)} \sum_k \sum_{\tilde{x}_{l-1,\tilde{x}_r}} \text{Tr} \left[ \hat{P} \left( \hat{A}_{k,B}^{(\tilde{x}_{l-1},\tilde{x}_r)} | \varphi \right)_{B} \right] M_{s_x}, \]

\[ := \frac{P(c)}{p(l)} \text{Tr} \left[ \hat{D}_{s_x|O_{l-1}} \hat{P} (|\phi(c)\rangle_B) \right]. \]

where

\[ \hat{D}_{s_x|O_{l-1}} = \sum_k \sum_{\tilde{x}_{l-1,\tilde{x}_r}} \hat{A}_{k,B}^{(\tilde{x}_{l-1},\tilde{x}_r)} M_{s_x} \hat{A}_{k,B}^{(\tilde{x}_{l-1},\tilde{x}_r)}. \]

Note that the discussions in the main text use the probability \( P(c) \) given in Eq. (A6) but do not employ the explicit form of \( \hat{D}_{s_x} \). Therefore, the relationships such as \( Y_{s_x,1s} = Y_{s_x,0s} + Y_{s_x,1s} - Y_{s_x,0s} \) that are considered in the main text can be interpreted as the linear relationships between the \( l \)th conditional probabilities \( Y_{s_x,c|O_{l-1}} \). This is so because the normalization factor \( p(l) \) of this interrelation. Thus, by taking the summation of such probabilities over \( l \), Azuma’s inequality [23, 24] gives the actual occurrence number of such events and the phase error rate in the virtual protocol can be estimated. This concludes the proof.

### Appendix B: Imperfect state preparation

In this section, we apply our phase error rate estimation technique to both a tilted four-state protocol, which is a variant of the BB84 scheme, and the three-state protocol with modulation errors. For the former, we assume that the terminal points of the four Bloch vectors associated with the four states sent by Alice form a triangular pyramid.

#### 1. A tilted four-state protocol

Here we show that is possible to obtain the precise detection rate of any state. Suppose that Alice sends Bob four states given by

\[ \hat{\rho}_{j\alpha} = \frac{1}{2} \left( \mathbb{1} + \sum_{l=x,y,z} p_{l\alpha} \hat{\sigma}_l \right), \]

where \( j \in \{0, 1\} \) and \( \alpha \in \{X, Z\} \). Moreover, let us assume that the vectors \( \tilde{V}_{j\alpha} \), with \( \tilde{V}_{j\alpha} = (1, p_{x\alpha}, p_{y\alpha}, p_{z\alpha}) \), are mutually linearly independent. From the viewpoint of the Bloch sphere, this means that the terminal points of the four Bloch vectors associated with the four states form a triangular pyramid. Suppose also that Alice and Bob distill key from the Z basis and use the events where Bob employs the X basis for parameter estimation. In this scenario, let \( |\phi_{j\alpha}\rangle_{A,B} \) denote a purification of \( \hat{\rho}_{j\alpha} \), with \( A \) and \( B \) representing, respectively, Alice’s shield system and the system that is sent to Bob. With this notation, Alice’s state preparation process in the Z basis can be described by using any of the following two source states,

\[ |\Psi_Z\rangle_{A,A_s,B} = \frac{1}{\sqrt{2}} \sum_{j=0,1} |j\rangle_A |\phi_{j\alpha}\rangle_{A_s,B}, \]

\[ |\Psi_Z\rangle_{A,A_s,B} = \frac{1}{\sqrt{2}} \sum_{j=0,1} |j\rangle_A |\phi_{j\alpha+1}\rangle_{A_s,B}, \]

where \( A \) is a virtual qubit system of Alice and the symbol \( \oplus \) denotes the modulo-2 addition. If Alice measures system \( A \) in the Z basis she prepares the desire state at site B, while she keeps the shield system \( A_s \). Here, the difference between Eqs. (B2) and (B3) is just a bit-flip. Since a bit-flip is a symmetry in the problem, Alice is allowed to choose any of the two equations above [Eqs. (B2) and (B3)] in constructing the purifications with the goal of optimising the key generation rate.

To calculate the phase error rate \( e_x \) we consider the virtual protocol where Alice and Bob measure \( |\Psi_Z\rangle_{A,A_s,B} \) in the X basis. In this virtual protocol, Alice emits

\[ \hat{\sigma}_{j\alpha|\text{Vir}} = \text{Tr}_{A,A_s} \left[ \hat{P} (|j\rangle_A) \otimes \text{I}_{A_s,B} \hat{P} (|\Psi_Z\rangle_{A,A_s,B}) \right]. \]

We denote these signals \( \hat{\sigma}_{j\alpha|\text{Vir}} \) as virtual states, and we define the normalised state \( \hat{\sigma}_{j\alpha|\text{Vir}} = \hat{\sigma}_{j\alpha|\text{Vir}} / \text{Tr}(\hat{\sigma}_{j\alpha|\text{Vir}}) \).
dependent, we can solve the set of linear equations given by Eq. (B2) or (B3). The phase error rate $e_x$ is given by

$$e_x = \frac{\dot{Y}_{0,x,0} + Y_{1,x,0}}{Y_{0,0,0} + Y_{1,0,0} + Y_{0,1,0} + Y_{1,1,0}}.$$  
(B4)

Now, since $\dot{\hat{Y}}_{B;\text{Vir}}$ can also be written as

$$\dot{\hat{Y}}_{B;\text{Vir}} = \frac{1}{2} \left( \hat{1} + \sum_{t=x,y,z} p_t^{V_\alpha,\text{Vir}} \hat{\sigma}_t \right),$$  
(B5)

to obtain $Y_{s,x;\text{Vir}}$ (and thus $e_x$) it is enough to calculate $q_{s,t} = \text{Tr}(\hat{D}_s \hat{\sigma}_t)/2$ with $t \in \{\hat{1}, x, y, z\}$. For this, note that in the actual experiment we have the following constraints,

$$Y_{s,x;\text{Vir}} = P(j_\alpha) \text{Tr} \left( \hat{D}_s \hat{\rho}_{j_\alpha} \right) = P(j_\alpha) \left( q_{s,0} \hat{1} + p_x^{j_\alpha} q_{s,x} + p_y^{j_\alpha} q_{s,y} + p_z^{j_\alpha} q_{s,z} \right).$$  
(B6)

Then, as long as the vectors $\vec{V}_{j_\alpha}$ are mutually linearly independent, we can solve the set of linear equations given by Eq. (B2) and obtain $q_{s,0} \hat{1}$, $q_{s,x}$, $q_{s,y}$, and $q_{s,z}$. That is, we can determine the exact transmission rate of any state, including the signal $\dot{\hat{Y}}_{B;\text{Vir}}$, which gives the phase error rate.

Moreover, if Bob’s POVM elements act on a qubit space and he performs a measurement in the Y-basis, Alice and Bob can also estimate the Y-basis error rate. To see this, note that one only needs to change in the discussion above the terms $s_x$ with $s_y$ and define the Y-basis virtual state as

$$\dot{\hat{Y}}_{B;\text{Vir}} = \text{Tr}_{A,A'} \left( \hat{P}(\vec{V}_{j_\alpha}) \otimes \hat{1}_{A',B} \hat{P} \left( |\Psi_Z\rangle_{A,A',B} \right) \right).$$

2. Three-state protocol

The technique described above can also be applied to the three-state protocol with modulation errors.

In particular, suppose that the corresponding vectors $\vec{V}_{j_\alpha}$ are mutually linearly independent and, moreover, the actual three states lie on the X-Z plane of the Bloch sphere. In this situation, we can consider the purifications given by Eq. (B2) or (B3) such that the coefficient $p_t^{V_\alpha,\text{Vir}} = 0$ in Eq. (B3). That is, all the coefficients of the purifications can be chosen to be real numbers in the X and Z bases. Now, since all the states, including the actual states and the virtual states, lie on the X-Z plane, we can obtain the transmission rate of the virtual states (and, consequently, the phase error rate $e_x$) by just using the same arguments provided in the main text.

This also implies that sending any three states, which do not necessarily lie on the X-Z plane, is enough to perform secure key distribution as long as the corresponding three vectors $\vec{V}_{j_\alpha}$ are mutually linearly independent. That is, the terminal points of the Bloch vectors associated with the three states form a triangle. This is so because all the states on the X-Z plane can be uniformly “lifted up” by a filtering operation $g(0_x)|0_x\rangle + (1-g)|1_x\rangle$ with $0 \leq g < 1$. That is, the virtual states can always be chosen on the same plane spanned by the three actual states. Thus, by using the transmission rate of the actual states, one can obtain the transmission rate of the virtual states and, therefore, also the phase error rate.

Appendix C: Simulation for the three-state protocol

In this section we present the calculations used to obtain Fig. 1 (a) in the main text. We begin with the single-photon components of the signals sent by Alice. In particular, we have that the single photon part of $|e^{i\theta_\alpha \sqrt{\alpha}}\rangle |e^{i\theta_\beta + \theta_\alpha \sqrt{\alpha} / \sqrt{2}}\rangle |0\rangle$ is given by $|1\rangle |0\rangle + e^{i(\theta_\alpha + \theta_\beta) / \sqrt{2}} |1\rangle$. Where 0 and 1 represent, respectively, the photon number. The set $\{(1,0), (0,1)\}$ forms a qubit basis. Therefore, we can choose the $Z$ basis such that Alice’s Z-basis states are expressed as

|φ_{0z}⟩ = |0_z⟩,
|φ_{1z}⟩ = \sin \frac{\delta}{2} |0_z⟩ + \cos \frac{\delta}{2} |1_z⟩,
(C1)

where $|0_y⟩ := |1_y⟩ |0_z⟩$ and $|1_y⟩ := |0_y⟩ |1_z⟩$ with $|0_z⟩ := (|0_y⟩ + |1_y⟩)/\sqrt{2}$ and $|1_z⟩ := (-i |0_y⟩ + i |1_y⟩)/\sqrt{2}$.

In the virtual protocol, Alice generates the state $|0_z⟩ |φ_{0z}⟩_B + |1_z⟩ |φ_{1z}⟩_B / \sqrt{2}$ and sends system B to Bob. This joint state can be equivalently expressed as

$$\sqrt{1 + \sin \frac{\delta}{2}} |0_z⟩_A |φ_{0z}⟩_B + \sqrt{1 - \sin \frac{\delta}{2}} |1_z⟩_A |φ_{1z}⟩_B,$$
(C2)

where the signals $|φ_{0z}⟩_B$ and $|φ_{1z}⟩_B$ have the form

|φ_{0z}⟩_B := C_{0,0}(\delta) |0_x⟩_B + C_{1,0}(\delta) |1_x⟩_B
|φ_{1z}⟩_B := C_{0,1}(\delta) |0_x⟩_B + C_{1,1}(\delta) |1_x⟩_B,
(C3)
(C4)

and the coefficients $C_{ij}(\delta)$ are given by

$$C_{0,0}(\delta) = \frac{1 + \sin \frac{\delta}{2} + \cos \frac{\delta}{2}}{2\sqrt{1 + \sin \frac{\delta}{2}}} + \frac{1 + \sin \frac{\delta}{2} - \cos \frac{\delta}{2}}{2\sqrt{1 - \sin \frac{\delta}{2}},
C_{0,1}(\delta) = \frac{1 - \sin \frac{\delta}{2} - \cos \frac{\delta}{2}}{2\sqrt{1 - \sin \frac{\delta}{2}}} + \frac{1 - \sin \frac{\delta}{2} + \cos \frac{\delta}{2}}{2\sqrt{1 + \sin \frac{\delta}{2}}},
C_{1,0}(\delta) = \frac{1 + \sin \frac{\delta}{2} + \cos \frac{\delta}{2}}{2\sqrt{1 + \sin \frac{\delta}{2}}} + \frac{1 + \sin \frac{\delta}{2} - \cos \frac{\delta}{2}}{2\sqrt{1 - \sin \frac{\delta}{2}},
C_{1,1}(\delta) = \frac{1 - \sin \frac{\delta}{2} - \cos \frac{\delta}{2}}{2\sqrt{1 - \sin \frac{\delta}{2}}} + \frac{1 - \sin \frac{\delta}{2} + \cos \frac{\delta}{2}}{2\sqrt{1 + \sin \frac{\delta}{2}}},$$

As already explained in the main text, our phase error rate estimation technique provides the exact value for the transmission rates $Y_{s,x;\text{Vir}}$. Therefore, we can obtain the precise transmission rate of the signals $|φ_{j\alpha}⟩_B$. 

For our simulations, we consider a channel model where the conditional probabilities $Y_{s_k|x}$ (i.e., the conditional probability that Bob obtains $s_k$ given that Alice sent him the state $|j_x\rangle$) are given by

$$Y_{s_k|x} = (1 - L)C_{s_k,j}(3\delta/2)^2(1 - e_d/2) + e_d(1 - e_d/2) + (1 - L)C_{s_j,j}(3\delta/2)^2e_d,$$  \hspace{1cm} (C5)

where $e_d$ is the dark count rate of Bob’s detectors, and $L$ denotes the total loss rate. Here, we have considered the transformation $\delta \rightarrow 3\delta/2$ because Bob applies a phase modulation to the incoming signals. In Eq. (C5), the first (second) term models a single detection click at Bob’s side produced by a photon (dark count), while the last term represents simultaneous clicks. Note that in this last case (simultaneous clicks), Bob assigns a random bit value to the measurement result.

For convenience, here we will write the phase error rate $e_x$ in terms of the conditional probabilities $Y_{s_k|x}$. Note that we can do so because the choice of the state and the measurement is random and uniform. We have that the phase error rate $e_x$ of the single-photon components, and the single-photon gain $Q_x$ are given by

$$e_x = \frac{Y_{1|0} + Y_{0|1}}{Y_{1|0} + Y_{0|1} + Y_{1|1} + Y_{0|0}}, \hspace{1cm} (C6)$$

$$Q_x = \frac{1}{2} - 2^{-\alpha} \sum_{x} Y_{s_k|x} P(j_x), \hspace{1cm} (C7)$$

where $P(j_x) = [1 + (-1)^j \sin(\delta/2)]/2$.

Similarly, one can obtain the overall gain $Q_z$ and the bit error rate $e_z$ in the $Z$ basis. These parameters have the form

$$e_z = w_z/Q_z,$$  \hspace{1cm} (C8)$$

$$Q_z = \frac{1}{2} \left[ P_{0|0}(1 - P_{1|0}) + (1 - P_{0|0})P_{1|0} + P_{0|1}P_{1|1} + P_{0|0}P_{1|1} \right],$$  \hspace{1cm} (C9)$$

$$w_z = \frac{1}{2} \left[ P_{0|0}(1 - P_{1|0}) + (1 - P_{0|0})P_{1|0} + P_{0|1}P_{1|1} \right],$$  \hspace{1cm} (C10)$$

where $P_{s|j}$ is the conditional probability that Bob obtains a bit value $s$ given that Alice sent him a bit value $j$. These probabilities can be written as

$$P_{0|0} = e_d + (1 - e_d) \left[ 1 - e^{-\alpha(1 - L)} \right],$$  \hspace{1cm} (C11)$$

$$P_{1|0} = e_d,$$  \hspace{1cm} (C12)$$

$$P_{0|1} = e_d + (1 - e_d) \left[ 1 - e^{-\alpha(1 - L)} \sin^2(\delta/2) \right],$$  \hspace{1cm} (C13)$$

$$P_{1|1} = e_d + (1 - e_d) \left[ 1 - e^{-\alpha(1 - L)} \cos^2(\delta/2) \right].$$  \hspace{1cm} (C14)$$

Finally, the asymptotic key generation rate is given by

$$R = \frac{1}{2} \left\{ Q_x \left[ 1 - h(e_x) \right] - Q_z h(e_z) \right\},$$  \hspace{1cm} (C15)$$

where $h(x)$ is the binary entropy function. For each value of the distance, we optimise the parameter $\alpha$ to maximise the key rate. The result is shown in Fig. 1 (a) in the main text.

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