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Clifford-group-restricted eavesdroppers in quantum key distribution

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Quantum key distribution (QKD) promises provably secure cryptography, even to attacks from an all-powerful adversary. However, with quantum computing development lagging behind QKD, the assumption that there exists an adversary equipped with a universal fault-tolerant quantum computer is unrealistic for at least the near-future. Here, we explore the effect of restricting the eavesdropper's computational capabilities on the security of QKD and find that improved secret key rates are possible. Specifically, we show that for a large class of discrete variable protocols higher key rates are possible if the eavesdropper is restricted to a unitary operation from the Clifford group. Further, we consider Clifford-random channels consisting of mixtures of Clifford gates. We numerically calculate a secret-key-rate lower bound for BB84 with this restriction and show that, in contrast to the case of a single restricted unitary attack, the mixture of Clifford-based unitary attacks does not result in an improved key rate.

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I. INTRODUCTION

Quantum key distribution (QKD) offers a potential path to quantum-safe cryptography that does not rely on the conjectured hardness of computational problems. An important problem in QKD is to devise a protocol that can be implemented using existing technology while maximizing the achievable secret key generation rate. QKD analyses have usually assumed that the eavesdropper is all-powerful: able to perform any quantum operation on the signals transferred between Alice and Bob. Such operations can, in principle, be implemented using a universal quantum computer along with a long-term quantum memory. This security without assumptions on the computational power of the adversary is one of the most compelling reasons to replace classical key exchange protocols with QKD [1,2].

Large-scale fault-tolerant quantum computers that can implement Shor's factoring algorithm [3] will render currently used classical cryptosystems such as the Rivest-Shamir-Adleman protocol [4], elliptic curve cryptography [5], and Diffie-Hellmann key exchange [6] insecure. Several classical cryptosystems, such as code-based encryption [7], lattice-based encryption [8], and supersingular isogenies [9], have been proposed as replacements for the Rivest-Shamir-Adleman protocol, and these post-quantum cryptosystems are based on hard problems that are conjectured to be difficult for quantum computers to solve efficiently [10]. As with all classical cryptosystems, proof of their security relies on the computational hardness of the underlying mathematical problem or, equivalently, on the computational power limitations of the adversary. In fact, there is so far no proof that guarantees

the nonexistence of an efficient quantum—or even classical—algorithm to break these post-quantum cryptosystems. Thus, in many real-world scenarios, the computational power of the adversary is the physically relevant condition.

While promising security without computational assumptions, in practice QKD protocols have been very challenging to implement, with successful demonstrations within a range of only a few hundred kilometers in optical fiber (see, e.g., [11–13]), and the rate without intermediate stations inevitably falls off with the transmittance of the channel [14]. Quantum repeaters [15–17] have been proposed as a way to improve key rates beyond the limitations of direct transmission [14,18]. While impressive progress has been made towards their demonstration, no such repeater has been realized [19]. However, assuming nothing about the nature of the adversary is overly pessimistic in the era of noisy intermediate-scale quantum (NISQ) computers [20]. Moreover, in the classical case, an eavesdropper can store the public information indefinitely and attack in the future when better algorithms or computational devices become available. In the quantum case, without a long-lived quantum memory, the eavesdropper must attack during the key exchange. Thus, for near-term QKD implementations the more relevant concern is the computational power of the eavesdropper *today*.

In this work, we examine the role that computational assumptions on the eavesdropper have on the secret key rate of discrete-variable quantum key distribution (DV-QKD) protocols. We examine the secret key rates that can be achieved if one restricts the eavesdropper to have access to a subclass of quantum operations formed by the Clifford group. Clifford operations are not universal and circuits built from them can be efficiently simulated classically [21], such that we would expect such a restriction to limit the power of the eavesdropper. We show that this is indeed the case for a large family

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of DV-QKD protocols. We then extend to Clifford-random channels, allowing the eavesdropper to implement a quantum channel described by a convex combination of unitary Clifford gates, and numerically calculate a lower bound to the secret key rate possible under this restriction for BB84 [22].

These restrictions are particularly relevant to practical QKD, as most candidate quantum computing architectures have demonstrated the ability to implement the full Clifford group with low error on physical qubits [23–27]. Thus, their implementation on logical qubits and fault-tolerant hardware is a much nearer-term reality than non-Clifford operations. A DV-QKD setup could realistically be attacked using either a Clifford restricted attack or a Clifford-random channel, as the only further resource required for this is classical randomness. Thus, the secret key rates calculated here are an upper bound for practical QKD, as they represent the absolute best-case scenario where the eavesdropper has as little computational power as can realistically be assumed for emerging quantum processors.

The problem of numerically computing the secret key rate can be cast as a nonlinear semidefinite program (SDP) [28,29]. In this framework, it becomes clear that the optimal attack an eavesdropper can use dictates the secret key rate that can be achieved. In particular, restricting the computational capabilities of the eavesdropper is equivalent to introducing further constraints to the key-rate SDP. To our knowledge, such computational assumptions on the eavesdropper and their impact on the secret key rate have not been considered in the literature.

Some work that is similar in spirit considers restrictions to the eavesdropper's ability to perform a coherent attack, due to either a noisy quantum memory used for storage [30] or general decoherence [31]. For these models, it has been shown that limiting the capabilities of the eavesdropper improves the key rate. Further, improved key rates can also be found when Eve's access to a wiretap channel is restricted, such as in a free-space communication setting where she can only collect a fraction of the transmitted optical signals [32].

II. RESULTS

A. Clifford-group restriction

We consider the broad class of prepare-and-measure QKD protocols from Ref. [33], for which the set of possible signal states consists of all elements from either 2, d , or $d+1$ mutually unbiased bases, where d (assumed prime) is the Hilbert space dimension of the signal-state system. Examples of QKD protocols contained in this class include BB84 [22] and the six-state protocol [34]. For these protocols, we assume that the eavesdropper Eve only has access to Bob's eventual half of the system and use a source-replacement scheme (see, e.g., [33], [35], [36]) to describe prepare-and-measure protocols as entanglement based. We are interested in Eve's optimal attack that minimizes the secret key rate.

The key observation in this section is that for the protocols described in Ref. [33], the state ρ_{AB} describing the optimal attack is also the Choi state describing the effective channel Eve implements on Bob's system. We can then ask what computational resources are required to simulate this effective

channel and determine if a restricted Eve can implement the optimal attack. We show that a Clifford-restricted Eve cannot implement the optimal attack in all situations. In the following we present our results, with details of the derivation contained in Appendix A.

The optimal attack for the protocols described in Ref. [33] leaves Alice and Bob's systems in a final state known as a *Bell-diagonal state*,

$$\rho_{AB} = \sum_{r,s}^{d-1} b_{r,s} |B_{r,s}^d\rangle\langle B_{r,s}^d|, \quad (1)$$

where $b_{r,s}$ are related to the bit-error rate and satisfy $\sum_{r,s}^{d-1} b_{r,s} = 1$ and $0 \leq b_{r,s} \leq 1$. Here $|B_{r,s}^d\rangle$ (see Appendix A) is a generalized Bell state. We now show how we can recast this expression in the form

$$\rho_{AB} = \rho_{\mathcal{E}_B} = \mathcal{I} \otimes \mathcal{E}_B(|B_{0,0}^d\rangle\langle B_{0,0}^d|), \quad (2)$$

where $\rho_{\mathcal{E}_B}$ is the Choi dual state describing the effective process on Bob's qubit due to Eve's interaction.

We recall that the Choi dual state of a quantum process $\mathcal{E}$ is defined by the action of the process on half of the maximally entangled state $|B_{0,0}^d\rangle$ [37]. Using that

$$|B_{r,s}^d\rangle = \hat{\mathbb{I}}_d \otimes \hat{P}_{r,s}^d |B_{0,0}^d\rangle, \quad (3)$$

where $\hat{P}_{r,s}^d$ are generalized Pauli matrices (see Appendix A), we rewrite the optimal attack as

$$\rho_{AB} = \sum_{r,s}^{d-1} b_{r,s} \hat{\mathbb{I}}_d \otimes \hat{P}_{r,s}^d |B_{0,0}^d\rangle\langle B_{0,0}^d| \hat{\mathbb{I}}_d \otimes (\hat{P}_{r,s}^d)^\dagger, \quad (4)$$

which has the desired form of a Choi dual state, demonstrating that $\rho_{AB} = \rho_{\mathcal{E}_B}$.

From here, it is straightforward to see that the effective channel $\mathcal{E}_B$ on Bob's system resulting from Eve's optimal attack is

$$\mathcal{E}_B(\rho_B) = \sum_{r,s}^{d-1} b_{r,s} \hat{P}_{r,s}^d \rho_B (\hat{P}_{r,s}^d)^\dagger. \quad (5)$$

We refer to this as a *Pauli-random channel*, as it is the convex combination of generalized Pauli operations. To simulate this effective channel requires only the ability to implement Pauli operators, together with a source of classical randomness.

The main result in this section is that even given an arbitrary finite number (N_E) of ancilla qudits, a Clifford-restricted Eve (acting with a Clifford gate on the joint system BE) cannot implement the optimal attack for all values of $b_{r,s}$, as she cannot simulate the effective channel of Eq. (5), without the source of classical randomness.

To see this, consider the Choi dual state for Eve's Clifford attack $\hat{U} \in \mathcal{C}\ell_d^{\otimes N_E+1}$ (see Appendix A for a definition of the Clifford group),

$$\rho_U = \hat{\mathbb{I}}_D \otimes \hat{U} |B_{0,0}^D\rangle\langle B_{0,0}^D| \hat{\mathbb{I}}_D \otimes \hat{U}^\dagger, \quad (6)$$

where $D = d^{N_E+1}$. One can easily show that the maximally entangled state for any dimension D can be written as the

following sum in the generalized Pauli basis

$$|B_{0,0}^D\rangle\langle B_{0,0}^D| = \frac{1}{D} \sum_{\substack{r, s, s' \\ s+s'=0 \bmod D}}^{D-1} \hat{P}_{r,s}^D \otimes \hat{P}_{r,s'}^D. \quad (7)$$

Putting this into Eq. (6) and using the fact the Clifford gates permute the members of the Pauli group, we have that

$$\rho_U = \frac{1}{D} \sum_{\substack{r, s, s' \\ s+s'=0 \bmod D}}^{D-1} e^{i\phi_{q(r,s')}} \hat{P}_{r,s}^D \otimes \hat{P}_{q(r,s')}^D, \quad (8)$$

where $q(r, s')$ describes the permutation action of the Clifford gate $\hat{U}$ and $\phi_{q(r,s')}$ describes the associated phase factor.

To determine the Choi dual state for the effective process on Bob's qudit alone, we take the partial trace with respect to all N_E of Eve's ancilla qubits on both D -dimensional subsystems of the Choi dual state [38]

$$\rho_{U_B} = \frac{1}{d} \sum_{n,m,j,k}^{d-1} \mu(n, m, j, k) \hat{P}_{n,m}^d \otimes \hat{P}_{j,k}^d, \quad (9)$$

where $\mu(n, m, j, k)$ is either 0 or a complex phase (see Appendix A for details).

The expression for ρ_{U_B} should be compared to the Choi dual state for the optimal attack channel given by Eq. (4), which can be rewritten in the Pauli basis as

$$\rho_{AB} = \sum_{r,s}^{d-1} \frac{b_{r,s}}{d} \sum_{\substack{n, k, k' \\ k+k'=0 \bmod d}}^{d-1} e^{i\phi_{q(r,s(n,k'))}} \hat{P}_{n,k}^d \otimes \hat{P}_{q(r,s(n,k'))}^d, \quad (10)$$

where we have used the fact that Pauli operators are themselves Clifford operators and so permute the elements of the Pauli group. Note that each term in the Pauli-random optimal attack channel results in a unique permutation, $q_{r,s}$, of the Pauli basis elements.

Equations (9) and (10) are in general inequivalent, as illustrated by the fact that each of the Pauli basis elements in ρ_{U_B} has a coefficient that has magnitude either 0 or $1/d$, while in ρ_{AB} the corresponding coefficient can have any complex value with a magnitude less than $1/d$ (determined by a sum of elements from the set $\{e^{i\phi_{q(r,s(n,k'))}} b_{r,s}\}$). Thus, except for specific values of $b_{r,s}$, Eve cannot simulate the optimal attack channel with only a Clifford gate and, so, cannot implement the optimal attack.

As a specific example, consider BB84, where the optimal attack channel is given by

$$\mathcal{E}_B(\rho_B) = (1-Q)^2 \hat{\mathbb{I}} \rho_B \hat{\mathbb{I}} + Q^2 \hat{Y} \rho_B \hat{Y} + Q(1-Q)(\hat{X} \rho_B \hat{X} + \hat{Z} \rho_B \hat{Z}), \quad (11)$$

with Q the average bit-error rate for all signal-state bases. For $Q = 0, 1$, or 0.5 , this effective channel can be implemented using a Clifford gate on BE , and we cannot rule out the possibility that restricted Eve can implement the optimal attack. For all other values of Q this is not the case. Note that for $Q = 0, 1$ the key rate is not reduced by Eve's interaction.

As Eq. (9) shows, a Clifford attack can be understood as a permutation of the Pauli basis operators of system B , along

with an acquired phase. For BB84, the two-qubit maximally entangled state can be written in the Pauli basis as

$$|B_{0,0}^2\rangle\langle B_{0,0}^2| = \frac{1}{4}(\hat{\mathbb{I}} \otimes \hat{\mathbb{I}} + \hat{X} \otimes \hat{X} - \hat{Y} \otimes \hat{Y} + \hat{Z} \otimes \hat{Z}),$$

and there are six allowed permutations of the Pauli operators on system B , with each element taking one of two phases (± 1). Not all 64 possibilities result in a valid density matrix, but for those that do we calculate the key rate and make comparisons to the worst case of Eq. (11), with Q determined from the output state of the Clifford attack channel. As expected, for $Q = 0, 1$, and 0.5 the Clifford and worst-case key rates are the same. For $Q = 0.25$ and 0.75 (the only other values possible for Clifford attacks), the Clifford attack key rate is finite, while the worst-case key rate is 0.

B. Clifford-random channel restriction

For the protocols we consider, we have shown that a Pauli-random channel describes the effective channel on Bob's qudit for the optimal eavesdropping attack and that this cannot be implemented by a Clifford gate on the combined system BE . However, this restriction may be seen as too severe, as with classical randomness but no additional quantum resources Eve can simulate a Pauli-random channel.

Given these facts, a natural relaxation for the eavesdropper restriction would be to give her the ability to use classical randomness to perform what we call Clifford-random channels,

$$\mathcal{E}(\rho) = \sum_{g \in \mathcal{C}^\ell} a_g \hat{\mathbb{I}}^A \otimes \hat{U}_g \rho \hat{\mathbb{I}}^A \otimes \hat{U}_g^\dagger, \quad (12)$$

where $\hat{U}_g$ is an $(N_E + 1)$ -qudit Clifford gate, and $\sum_g a_g = 1$, of which Pauli-random channels are a subset. Practically, such a channel can be implemented by Eve if she acts with a random Clifford gate on each signal state she intercepts. This requires only the ability to implement Clifford gates, plus a source of classical randomness, such as a coin.

Given such a capability, the eavesdropper can directly implement the effective channel of Eq. (5) and *simulate* the statistics of the optimal attack. However, this does not mean that the eavesdropper can implement the optimal attack that gives her the most information. As such, we wish to quantify how much information a Clifford-random channel restricted Eve can obtain, by determining a lower bound to the secret key rate for this restriction. To do so, we use the numerical optimization approach developed in Refs. [28] and [29], where a computational restriction on the eavesdropper will introduce constraints to the optimization, shrinking the feasible set of states ρ_{AB} describing the optimal attack.

Let us denote the combined state of ABE after the Clifford-random channel as ρ_{ABE} , which will in general be a mixed state. We introduce an auxiliary Hilbert space F that is sufficiently large to purify ρ_{ABE} into the pure state ρ_{ABEF} . Using the results in Refs. [28] and [39], it is straightforward to see that the secret key rate is given by the expression

$$k(\rho_{ABF}) = r(\rho_{ABF}) - p_{\text{pass}} \text{leak}_{\text{EC}}, \quad (13)$$

$$r(\rho_{ABF}) = D(\mathcal{G}(\rho_{ABF}) || \mathcal{Z}^R(\mathcal{G}(\rho_{ABF}))),$$

where $D(\rho || \sigma) = \text{Tr}[\rho(\log_2 \rho - \log_2 \sigma)]$ is the quantum relative entropy.

As described in detail in Ref. [29], $\mathcal{G}(\cdot)$ is a completely positive trace-nonincreasing quantum channel that describes the measurements, public announcements, and postselection performed by Alice and Bob, with p_{pass} the probability that the postselection is successful. The term leak_{EC} describes the information leaked (and available to the eavesdropper) during the error correction used to generate a secure key, and $\mathcal{Z}^R(\cdot)$ is a pinching channel over the Hilbert space R that records the results of Alice's key map,

$$\mathcal{Z}^R(\rho) = \sum_i |i\rangle\langle i|^R \rho |i\rangle\langle i|^R, \quad (14)$$

where $\{|i\rangle_R\}$ is an orthonormal basis for R .

To find a lower bound for the key rate, we would solve the nonlinear semidefinite program, defined in Ref. [29], that finds the state ρ_{ABF}^* that minimizes $r(\rho_{ABF})$ from Eq. (13), taking into account constraints on the final state ρ_{ABF} that come from channel reconciliation, such as the quantum bit-error rate. Unfortunately, without knowledge of the nature of F , we cannot calculate Eq. (13) and, thus, cannot evaluate the cost function of our SDP.

However, using the monotonicity of the quantum relative entropy under completely positive and trace-preserving maps, we have that

$$D(\mathcal{G}(\rho_{ABF}^*) || \mathcal{Z}^R(\mathcal{G}(\rho_{ABF}^*))) \geq D(\mathcal{G}(\rho_{AB}^*) || \mathcal{Z}^R(\mathcal{G}(\rho_{AB}^*))),$$

where $\rho_{AB}^* = \text{Tr}_F[\rho_{ABF}^*]$. Using this, clearly

$$r(\rho_{ABF}^*) \geq r(\rho_{AB}^*) \geq r(\rho'_{AB}), \quad (15)$$

with ρ'_{AB} the optimal solution for a key-rate SDP over states in AB . It is straightforward to modify the SDP in Ref. [29] to include constraints from restricted Eve (see Appendices B and C for details), and thus we can numerically find a *lower bound* to the key rate for the optimal Clifford-random channel attack.

In practice, numerical SDP solvers are not able to return the exact optimal solution ρ'_{AB} . Solving the primal problem of the SDP will in general give an upper bound to the optimum, so instead we solve the dual problem, which gives a lower bound. This guarantees that $r(\rho'_{AB})$ is a lower bound to the secret key rate. To solve the dual problem we use the convex approximation to the quantum relative entropy developed in [40], which integrates with CVX, a MATLAB package for specifying and solving convex problems [41,42]. In Appendix F we discuss how to obtain a *secure* lower bound using the techniques from either Ref. [40] or Ref. [29] and present numerical evidence that our approximate lower bounds are accurate to a high precision.

C. Clifford-random channel restricted BB84

As an example of our numerical approach, we consider prepare-and-measure BB84, with the modification that we allow the initial state to be any state of the form

$$|\Psi_I\rangle_{AA'} = \sqrt{b}|00\rangle + \sqrt{1-b}|11\rangle, \quad (16)$$

where $0 \leq b \leq 1$. After Alice prepares this initial state, she sends the second register A' to Bob via the insecure quantum channel that Eve has access to, and we call the register after the transmission B . For $b \neq 1/2$ these initial states lead to BB84 protocols that we refer to as asymmetric.

The protocol we consider is outlined as follows (details can be found in Appendix D).

1. Alice and Bob each independently measure in the Z basis or X basis, with probability p and $1 - p$, respectively.
2. Alice's key map maps the $+1$ measurement outcome to the character 0 and the -1 outcome to the character 1, i.e.,

$$\{|0\rangle, |+\rangle\} \rightarrow 0, \quad \{|1\rangle, |-\rangle\} \rightarrow 1, \quad (17)$$

where $|\pm\rangle \propto |0\rangle \pm |1\rangle$ are the eigenstates of $\hat{X}$.

3. Alice and Bob perform channel reconciliation, which adds one of two sets of constraints to the SDP, both of which can be calculated from asymptotic measurement statistics.

a. Coarse-grained constraints:

$$\text{Tr}[\rho_{AB} \hat{E}_{Z/X}] = \gamma_{z/x}, \quad (18)$$

where

$$\hat{E}_Z = |01\rangle\langle 01| + |10\rangle\langle 10|, \quad (19)$$

$$\hat{E}_X = |+-\rangle\langle +-| + |-+\rangle\langle -+|. \quad (20)$$

b. Fine-grained constraints:

$$\text{Tr}[\rho_{AB} \hat{E}_{ij}] = \gamma_{ij}, \quad (21)$$

where

$$\hat{E}_{ij} = \hat{M}_i \otimes \hat{M}_j \quad (22)$$

with $\hat{M}_i \in \{|0\rangle\langle 0|, |1\rangle\langle 1|, |+\rangle\langle +|, |-\rangle\langle -|\}$.

4. Further constraints to the SDP come from the complete knowledge of Alice's reduced state, to which Eve does not have access, and from our knowledge of Eve's restriction.

We simulate data to calculate the constraints and the error correction cost leak_{EC} using a depolarizing channel with depolarizing probability ϵ (see Appendix E for further details). For our input state on AA' , this produces an output state on AB given by

$$\mathcal{E}_{\text{dep}}(\rho_{AA'}) = (1 - \epsilon)\rho_{AA'} + \epsilon \text{Tr}_B[\rho_{AA'}] \otimes \frac{1}{2}\hat{1}^B, \quad (23)$$

where $\rho_{AA'}$ is the pure state of Eq. (16). We alternatively refer to ϵ as the channel error, as it is the error added to the state by the insecure channel between Alice and Bob.

The results of our numerical calculations of key-rate lower bounds for a Clifford-channel restricted Eve are shown in Fig. 1. These are compared with the key rates for an unrestricted Eve (we solve both the primal and the dual problem and find a duality gap much smaller than our reported key rate). Figure 1(a) shows the key-rate lower bound for an asymmetric initial state ($b = 1/9$) as a function of the channel error ϵ , while Fig. 1(b) varies the asymmetry parameter b and keeps the channel error fixed at $\epsilon = 0.1$. In both cases the probability that either Alice or Bob measures in the Z basis is $p = 0.5$.

As both plots show, the comparison between the restricted and the unrestricted key rates depends strongly on the constraints used in the SDP, i.e., on how much characterization Alice and Bob do of the insecure channel connecting them. For the coarse-grained constraints the restricted key-rate lower bound can be significantly larger than the unrestricted key rate (depending on the asymmetry), while for the fine-grained

FIG. 1. Secret-key-rate lower-bound function as a function of (a) channel error ϵ and (b) asymmetry parameter b , with or without a restricted eavesdropper and with either coarse- or fine grained constraints. For the restricted eavesdropper the key rate is the same for both sets of constraints. Fixed parameters indicated in each plot.

constraints they are identical (note that the restricted key-rate lower bound is the same regardless of the constraints). This result is unsurprising, as from the perspective of SDP optimization, restricting Eve is equivalent to adding additional constraints. It turns out that for BB84 the additional constraints coming from a restricted Eve can also be determined by fine-grained channel reconciliation. In fact, we can determine that it is the constraint

$$\begin{aligned} \gamma_{IZ} &= \langle \hat{I}^A \otimes \hat{Z}^B \rangle_{\rho_{AB}} = \sum_{n,k=0}^1 (-1)^k \langle n, k | \rho_{AB} | n, k \rangle \\ &= \gamma_{00} - \gamma_{01} + \gamma_{10} - \gamma_{11} \end{aligned} \quad (24)$$

provided by both restricted Eve and the fine-grained constraints that is responsible.

III. DISCUSSION

In this paper, we have studied the role of the computational capabilities of the eavesdropper in the secret key rates achievable for a QKD protocol. Specifically, for discrete-variable protocols with d mutually unbiased bases and Weyl-Heisenberg symmetry, we found that the optimal attack

for the eavesdropper cannot be implemented by a single Clifford gate with even an arbitrary number of ancilla qudits given to the eavesdropper. In the specific case of BB84, finite key rates are possible for a Clifford-gate restricted eavesdropper when the worst-case attack has zero key rate.

We then considered Clifford-random channels and derived a way to use the numerical approach in Ref. [29] to find a lower bound for eavesdropper attacks with a total final state that is mixed. Again for BB84, we calculated the secret key rate with a Clifford-random channel restricted eavesdropper by modifying the SDP to incorporate the restriction. To do so, we have developed several reductions to the QKD numerical SDP problem to make it computationally tractable, generalizations of which may find use in other numerical studies of QKD protocols (see Ref. [43] and Appendix D for further details). We found that the difference between the worst-case Clifford-random channel restricted key rate and the optimal attack key rate depends on the information obtained during channel reconciliation.

For BB84 we found that a Clifford-random channel restriction does not reveal any information about the channel not available from full channel reconciliation, and there is no key-rate improvement for a restricted eavesdropper. However, we have only calculated a lower bound to the key rate, due to our inability to describe the purifying system F . To calculate the key rate, or bound it more tightly, future research is needed to develop methods for calculating secret key rates with mixed final states (where the problem cannot be cast in terms of the quantum relative entropy) or that incorporate the purifying auxiliary system [44,45].

Further, while we have not shown an improved key-rate lower bound for Clifford-random channel restricted BB84, we have analytically shown an improved key rate for Clifford-gate restricted BB84. Thus, we anticipate that numerical approaches similar to ours will find improved key rates for other restrictions and other protocols, especially those with systems in larger Hilbert spaces. We intend our work to serve as the initiation point for the general study of QKD with computational restrictions. This will be especially relevant in the near term, where QKD technological development is likely to outpace the development of universal quantum computers.

We have studied restrictions involving Clifford gates, as these are most likely to be fault-tolerantly implementable in the near-future (e.g., on the surface code [46]) and can be implemented transversally, i.e., in a parallel fashion. Further, they are analogous to Gaussian operations in the continuous-variable (CV) case, which can be implemented with only linear optics and, hence, provide a reasonable model for restrictions on the eavesdropper for CV systems. Future work will seek to generalize the study of computational restrictions to such CV-QKD protocols and to implementations of DV-QKD using weak coherent states.

Finally, we note that computational restrictions are an assumption that QKD users may choose to make about the eavesdropper. If the measurement results contain evidence that the eavesdropper is restricted, then the standard security proof formalism will produce a secret key rate that takes this into account, and such assumptions are not necessary. In this work, we have focused on the situation where a restricted

eavesdropper cannot be inferred from the measurement results and shown how to add the assumption of a restricted eavesdropper into a numerical security proof formalism.

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APPENDIX A: DERIVATION OF THE CLIFFORD-GATE EFFECTIVE CHANNEL

The generalized Bell states for two qudits are

$$|B_{r,s}^d\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} e^{\frac{2\pi i}{d} ks} |k\rangle |k+r\rangle, \quad (\text{A1})$$

and the generalized Pauli matrices of dimension d are

$$\hat{P}_{r,s}^d = \sum_{k=0}^{d-1} e^{\frac{2\pi i}{d} ks} |k+r\rangle \langle k+r| k. \quad (\text{A2})$$

The generalized Pauli matrices form a group, $\mathcal{P}_d$, and the Clifford group of dimension d , $\mathcal{C}\ell_d$, is the set of unitary operations that map the Pauli group to itself under conjugation, i.e.,

$$\hat{U} \in \mathcal{C}\ell_d \quad \text{iff} \quad \hat{U} \mathcal{P}_d \hat{U}^\dagger = \mathcal{P}_d. \quad (\text{A3})$$

Note that the action of a Clifford-group element on the Pauli group induces a distinct complex phase factor to each element in the Pauli group. For $d = 2^n$ this phase factor is ± 1 .

From Eq. (8), deriving the Choi state for the effective process on Bob's qudit alone is done by taking the partial trace of Eve's N_E ancilla qubits as

$$\begin{aligned} \rho_{U_B} &= \frac{1}{D} \sum_{\substack{r, s, s' \\ s+s'=0}}^{D-1} e^{i\phi_{q(r,s')}} \text{Tr}_{1\dots N_E} [\hat{P}_{r,s}^D] \otimes \text{Tr}_{1\dots N_E} [\hat{P}_{q(r,s')}^D] \\ &= \frac{1}{d} \sum_{n,m,j,k} \mu(n, m, j, k) \hat{P}_{n,m}^d \otimes \hat{P}_{j,k}^d, \end{aligned} \quad (\text{A4})$$

where, for brevity, when we write $s + s' = 0$ it should be understood that this is addition modulo D . To arrive at the last line we have used the facts that

$$\text{Tr}[\hat{P}_{r,s}^d] = d\delta_{r,0}\delta_{s,0} \quad (\text{A5})$$

and that a d^{N_E} -dimensional Pauli operator is a tensor product of N_E d -dimensional Pauli operators. The complex weight function $\mu(n, m, j, k)$ is 0 unless

$$\hat{P}_{r,s}^D = \hat{\mathbb{I}}_d^{\otimes N_E} \otimes \hat{P}_{n,m}^d \quad \text{and} \quad \hat{P}_{q(r,s')}^D = \hat{\mathbb{I}}_d^{\otimes N_E} \otimes \hat{P}_{j,k}^d \quad (\text{A6})$$

can be satisfied simultaneously for some valid r, s , and s' , in which case it takes the value of $e^{i\phi_{q(r,s')}}$.

APPENDIX B: SEMIDEFINITE PROGRAM SETUP FOR BB84

With no restriction on the eavesdropper, there is no need to introduce the auxiliary system F , and we can directly solve an SDP for ρ_{AB} [29]. We solve the SDP

$$\begin{aligned} \min_{\rho_{AB}} & (p^2 D(\rho_{AB} || \mathcal{Z}_Z^A(\rho_{AB})) + (1-p)^2 D(\rho_{AB} || \mathcal{Z}_X^A(\rho_{AB}))), \\ \rho_{AB} & \geq 0, \quad \text{Tr}(\rho_{AB}) = 1, \\ \text{Tr}(\rho_{AB} \hat{E}_{Z/X}) &= \gamma_{z/x} \quad \text{or} \quad \text{Tr}(\rho_{AB} \hat{E}_{ij}) = \gamma_{ij}, \\ \langle \hat{X}^A \rangle_{\rho_{AB}} &= \langle \hat{Y}^A \rangle_{\rho_{AB}} = 0, \quad \langle \hat{Z}^A \rangle_{\rho_{AB}} = 2b^2 - 1, \end{aligned}$$

where the minimization is over $\rho_{AB} \in \mathcal{B}(\mathcal{H}_{AB})$. The second line of constraints implements either the coarse- or the fine-grained constraints from channel reconciliation. Here $\mathcal{Z}_\mu^K(\cdot)$ is the pinching channel on Hilbert space K in the basis of the operator $\hat{\mu}$. The derivation of this SDP can be found in Ref. [29], except for the separation of the objective function into two parts, which can be found in Appendix D. This separation enables all operations to be on the AB Hilbert space alone. The last line of constraints comes from the complete knowledge of the reduced state of Alice, where we have used the shorthand

$$\langle \hat{\mu}^A \rangle_{\rho_{AB}} = \text{Tr}(\rho_{AB} \hat{\mu} \otimes \hat{\mathbb{I}}) \quad (\text{B1})$$

for compactness.

A restriction on Eve's computational power places additional constraints in this optimization problem, which reduces the set of feasible ρ_{AB} . As such we can augment the SDP written above with additional constraints on ρ_{AB} that encode how the set of operations the eavesdropper can perform is restricted. However, for our Clifford-random channel restriction we find it simpler to introduce a parametrization of ρ_{AB} in the feasible set in a smart choice of matrix basis, as it is not straightforward to construct additional constraints of the standard form used in [29]. Some of the coefficients in this parametrization are constrained optimization parameters, which we label C_μ^j .

For a Clifford-random channel restricted eavesdropper, we solve the SDP

$$\begin{aligned} \min_{C_\mu^j \in \mathbb{R}} & r(\rho_{AB}[C_\mu^j]), \\ \rho_{AB} & \geq 0, \\ \text{Tr}(\rho_{AB} \hat{E}_{Z/X}) &= \gamma_{z/x} \quad \text{or} \quad \text{Tr}(\rho_{AB} \hat{E}_{ij}) = \gamma_{ij}, \\ \sum_{j,\mu} C_\mu^j &= 3, \quad \sum_{\mu} C_\mu^j \leq 1 \forall j, \quad 0 \leq C_\mu^j \leq 1, \end{aligned}$$

where $\rho_{AB}[C_\mu^j]$ is the state written in our chosen matrix basis, with free parameters C_μ^j . For compactness of notation we have suppressed the functional dependence of ρ_{AB} on the free parameters C_μ^j below the first line. The function $r(\rho_{AB}[C_\mu^j])$ is the same as in the unrestricted SDP, but with ρ_{AB} replaced by $\rho_{AB}[C_\mu^j]$. The optimization domain becomes the real numbers for the free parameters C_μ^j .

The parameterized $\rho_{AB}[C_\mu^j]$ lies within a subset of the Hermitian, trace 1 matrices, defined by additional constraints

coming from the eavesdropper's restriction to Clifford-random channels. The complete knowledge of Alice's reduced state is also encoded in this parametrization, so those constraints are not added to the SDP as they are in the unrestricted case. A complete description of the parametrization of $\rho_{AB}[C_\mu^j]$ and its derivation can be found in Appendix C.

Both SDPs require optimizations over density matrices within the AB Hilbert space alone. However, unlike in the standard problem setup [29], we have derived an SDP where the operations performed on ρ_{AB} do not require dilation to a larger Hilbert space that includes descriptions of measurement outcomes, public announcements, and postselection. For instance, the pinching channels are on the Hilbert space A instead of R . This greatly improves the numerical performance of the optimization. A detailed description of how we have reduced the operational Hilbert space dimension of the secret-key-rate function can be found in Appendix D and is related to techniques used in [43].

APPENDIX C: RESTRICTED EAVESDROPPER FOR QUBIT SYSTEMS

1. General setup

In a prepare-and-measure setup, via a source replacement scheme we can describe the initial state of Alice and Bob as

$$|\Psi_I\rangle_{AA'} = \sum_n \sqrt{p_n} |n\rangle |\phi_n\rangle, \quad (C1)$$

where Alice records the choice of the state she prepares in register A and sends the state in register A' to Bob, which becomes system B after the channel controlled by Eve. The full initial state of Alice, Bob, and Eve is

$$|\Psi_I\rangle_{AA'E} = |\Psi_I\rangle_{AA'} |0\rangle^{\otimes N_E}, \quad (C2)$$

where assuming that Eve's initial state is pure, we can with complete generality define it to be the product state of all Eve's ancilla qubits in state $|0\rangle$. Eve can act only on the A' half of the initial AA' state, as well as her own state. Assuming that Eve implements the unitary $\hat{U} \in B(\mathcal{H}_{A'} \otimes \mathcal{H}_E)$, which is a general description for Eve's attack under the i.i.d. assumption we have made, then the final state of ABE is given by

$$\rho_{ABE} = \hat{U} |\Psi_I\rangle\langle\Psi_I|_{AA'E} \hat{U}^\dagger. \quad (C3)$$

The state of AB alone is $\rho_{AB} = \text{Tr}_E(\rho_{ABE})$, which we parametrize as

$$\rho_{AB} = \sum_i \gamma_i \hat{\Gamma}_i + \sum_j \omega_j \hat{\Omega}_j. \quad (C4)$$

Here $\hat{\Gamma}_i$ are the operators whose expectation value with state ρ_{AB} is known, either through the complete knowledge of the state of A , $\rho_A = \text{Tr}_E(\rho_{ABE})$, or from parameter estimation. The set $\hat{\Omega}_j$ completes an orthonormal basis for operator space and has unknown expectation values given by

$$\begin{aligned} \omega_j &= \text{Tr}(\rho_{AB} \hat{\Omega}_j) = \text{Tr}(\hat{U} |\Psi_I\rangle\langle\Psi_I|_{ABE} \hat{U}^\dagger \hat{\Omega}_j) \\ &= \langle\Psi_I|_{ABE} \hat{U}^\dagger \hat{\Omega}_j \hat{U} |\Psi_I\rangle_{ABE} \equiv \langle\hat{U}^\dagger \hat{\Omega}_j \hat{U}\rangle, \end{aligned} \quad (C5)$$

where the last expression is a notational definition we use for convenience.

2. Restriction to Clifford operations

Let us assume that Eve can only implement Clifford gates on the combined system BE . Then it is smart to choose $\hat{\Gamma}_i$ and $\hat{\Omega}_j$ to be Pauli operators. In Eq. (C5) we consider the full system ABE , and so append the identity operator acting on Eve's system to $\hat{\Gamma}_i$ and $\hat{\Omega}_j$, such that we set

$$\hat{\Gamma}_i = \hat{P}_i^A \otimes \hat{P}_i^B \otimes \hat{\mathbb{I}}^{\otimes N_E}, \quad (C6)$$

$$\hat{\Omega}_j = \hat{P}_j^A \otimes \hat{P}_j^B \otimes \hat{\mathbb{I}}^{\otimes N_E}, \quad (C7)$$

with $\hat{P}_j^A, \hat{P}_j^B \in \frac{1}{\sqrt{2}}\{\hat{\mathbb{I}}, \hat{X}, \hat{Y}, \hat{Z}\}$ normalized single-qubit Pauli operators. The restriction to Clifford operations is such that Eve can only implement a unitary $\hat{U}_g \in \mathcal{C}\ell(\mathcal{H}_{A'} \otimes \mathcal{H}_E)$, and the operation on the full Hilbert space ABE is given by

$$\hat{U} = \hat{\mathbb{I}}^A \otimes \hat{U}_g. \quad (C8)$$

As Clifford operations map Pauli matrices to other Pauli matrices, we see that

$$\omega_j = \langle(\hat{\mathbb{I}}^A \otimes \hat{U}_g^\dagger) \hat{\Omega}_j (\hat{\mathbb{I}}^A \otimes \hat{U}_g)\rangle = \langle\pm \hat{\Omega}_j^{(g)}\rangle, \quad (C9)$$

where $\hat{\Omega}_j^{(g)} = \hat{P}_j^A \otimes \hat{P}_j^B$, with $\hat{P}_j^{(g)} = \pm \hat{U}_g^\dagger (\hat{P}_j^A \otimes \hat{\mathbb{I}}^{\otimes N_E}) \hat{U}_g$ an $(N_E + 1)$ -qubit Pauli operator. Note that the $\pm$ sign in the expectation value is meant to imply that, depending on the Clifford gate $\hat{U}_g$, we may have either $+\hat{\Omega}_j^{(g)}$ or $-\hat{\Omega}_j^{(g)}$.

Extending to Clifford-random channels, Eve's action is generically described by

$$\rho_{ABE} = \sum_{g \in \mathcal{C}\ell} a_g \hat{\mathbb{I}}^A \otimes \hat{U}_g |\Psi_I\rangle\langle\Psi_I|_{AA'E} \hat{\mathbb{I}}^A \otimes \hat{U}_g^\dagger, \quad (C10)$$

with $\sum_g a_g = 1$. Then for the unknown parameters ω_j we have

$$\omega_j = \sum_g a_g \langle(\hat{\mathbb{I}}^A \otimes \hat{U}_g^\dagger) \hat{\Omega}_j (\hat{\mathbb{I}}^A \otimes \hat{U}_g)\rangle, \quad (C11)$$

where, as a reminder, $\hat{\Omega}_j$ is a two-qubit Pauli operator on AB (dilated to account for E). To make this more explicit, we define

$$\begin{aligned} \omega_j^k &= \sum_g a_g \langle(\hat{\mathbb{I}}^A \otimes \hat{U}_g^\dagger) \hat{P}_k^A \otimes \hat{P}_j^B \otimes \hat{\mathbb{I}}^{\otimes N_E} (\hat{\mathbb{I}}^A \otimes \hat{U}_g)\rangle \\ &= \sum_g a_g \langle\hat{P}_k^A \otimes \hat{P}_{j,g}^B \otimes \hat{P}_{j,g}^E\rangle, \end{aligned} \quad (C12)$$

where we have defined

$$\hat{P}_{j,g}^B \otimes \hat{P}_{j,g}^E = \hat{U}_g^\dagger (\hat{P}_j^B \otimes \hat{\mathbb{I}}^{\otimes N_E}) \hat{U}_g, \quad (C13)$$

with $\hat{P}_{j,g}^E$ an N_E -qubit Pauli matrix that is *not* normalized. From here, the first key observation is that since Eve's initial state is $|0\rangle^{\otimes N_E}$, only those N_E -qubit Pauli operators contained within the set $\hat{P}_{j,g}^E \in \{\hat{\mathbb{I}}, \hat{Z}\}^{\otimes N_E}$ have a nonzero expectation value with Eve's initial state. Thus we have that

$$\langle\hat{P}_{j,g}^E\rangle = 0 \quad \text{or} \quad \pm 1 \quad (C14)$$

and we can rewrite Eq. (C12) as

$$\begin{aligned} & \sum_g a_g \langle \hat{P}_k^A \otimes \hat{P}_{j,g}^B \otimes \hat{P}_{j,g}^E \rangle \\ &= \sum_g a_g \langle \hat{P}_k^A \otimes \hat{P}_{j,g}^B \rangle \langle \hat{P}_{j,g}^E \rangle \\ &= \sum_{g_+^j} a_{g_+^j} \langle \hat{P}_k^A \otimes \hat{P}_{j,g}^B \rangle - \sum_{g_-^j} a_{g_-^j} \langle \hat{P}_k^A \otimes \hat{P}_{j,g}^B \rangle. \end{aligned} \quad (\text{C15})$$

The last expression not only splits the summation into two parts but drops all a_g with $\langle \hat{P}_{j,g}^E \rangle = 0$, and so the sum of the remaining a_g may be less than 1.

Further, we know that for $\hat{P}_j^B \neq \hat{I}/\sqrt{2}$, the action of $\hat{U}_g$ can only transform $\hat{P}_j^B$ such that $\hat{P}_{j,g}^B \in \frac{1}{\sqrt{2}}\{\hat{X}, \hat{Y}, \hat{Z}\}$. This allows us to split Eq. (C12) into six separate sums, distinguished by $\hat{P}_{j,g}^B$ and Eq. (C15),

$$\begin{aligned} \sqrt{2}\omega_j^k &= \sum_{g_X^j} a_{g_X^j} \langle \hat{P}_k^A \otimes \hat{X}^B \rangle + \sum_{g_Y^j} a_{g_Y^j} \langle \hat{P}_k^A \otimes \hat{Y}^B \rangle \\ &+ \sum_{g_Z^j} a_{g_Z^j} \langle \hat{P}_k^A \otimes \hat{Z}^B \rangle - \sum_{g_{-X}^j} a_{g_{-X}^j} \langle \hat{P}_k^A \otimes \hat{X}^B \rangle \\ &- \sum_{g_{-Y}^j} a_{g_{-Y}^j} \langle \hat{P}_k^A \otimes \hat{Y}^B \rangle - \sum_{g_{-Z}^j} a_{g_{-Z}^j} \langle \hat{P}_k^A \otimes \hat{Z}^B \rangle, \end{aligned} \quad (\text{C16})$$

where now the summation index g_μ^j , for $\hat{\mu} \in \{\hat{X}, \hat{Y}, \hat{Z}\}$, runs over all $(N_E + 1)$ -qubit Clifford gates that transform $\hat{P}_j^B$ of Eq. (C12) such that $\sqrt{2}\hat{P}_j^B \otimes \hat{I}^{\otimes N_E} \rightarrow \hat{\mu} \otimes \hat{P}_g^E$, with

$$\hat{\mu} \in \{\hat{X}, \hat{Y}, \hat{Z}\} \quad \text{and} \quad \hat{P}_g^E \in \{\hat{I}, \hat{Z}\}^{\otimes N_E} \text{ s.t. } \langle \hat{P}_g^E \rangle = 1$$

or

$$\hat{\mu} \in -\{\hat{X}, \hat{Y}, \hat{Z}\} \quad \text{and} \quad \hat{P}_g^E \in \{\hat{I}, \hat{Z}\}^{\otimes N_E} \text{ s.t. } \langle \hat{P}_g^E \rangle = -1,$$

which gives a plus sign to the coefficient $a_{g_\mu^j}$, and the summation index $g_{-\mu}^j$ runs over all $(N_E + 1)$ -qubit Clifford gates that transform $\hat{P}_j^B$ as before but with

$$\hat{\mu} \in -\{\hat{X}, \hat{Y}, \hat{Z}\} \quad \text{and} \quad \hat{P}_g^E \in \{\hat{I}, \hat{Z}\}^{\otimes N_E} \text{ s.t. } \langle \hat{P}_g^E \rangle = 1$$

or

$$\hat{\mu} \in \{\hat{X}, \hat{Y}, \hat{Z}\} \quad \text{and} \quad \hat{P}_g^E \in \{\hat{I}, \hat{Z}\}^{\otimes N_E} \text{ s.t. } \langle \hat{P}_g^E \rangle = -1,$$

which gives a minus sign to the coefficient $a_{g_{-\mu}^j}$.

We have only considered $j = 1, 2, 3$, which corresponds to $\hat{P}_j^B \in \frac{1}{\sqrt{2}}\{\hat{X}, \hat{Y}, \hat{Z}\}$, as for $\hat{P}_0^B = \hat{I}/\sqrt{2}$ the expressions for ω_0^k are trivially given by

$$\begin{aligned} \omega_0^k &= \frac{1}{\sqrt{2}} \sum_g a_g \langle (\hat{I}^A \otimes \hat{U}_g) \hat{P}_k^A \otimes \hat{I}^B \otimes \hat{I}^{\otimes N_E} (\hat{I}^A \otimes \hat{U}_g^\dagger) \rangle \\ &= \frac{1}{\sqrt{2}} \langle \Psi_I |_{AA'} \hat{P}_k^A \otimes \hat{I}^B | \Psi_I \rangle_{AA'} \end{aligned} \quad (\text{C17})$$

and describe the initial state of A .

The summations in Eq. (C16) separate the Clifford group into disjoint subsets defined by the action of its elements on a Pauli operator $\hat{P}_j^B$, and therefore the sets of free parameters $\{a_{g_\mu^j}\}$ are disjoint for a given j . For each summation, we can

therefore define

$$C_v^j = \sum_{g_v^j} a_{g_v^j} \quad (\text{C18})$$

and rewrite Eq. (C16) as

$$\begin{aligned} \sqrt{2}\omega_j^k &= C_X^j \langle \hat{P}_k^A \otimes \hat{X}^B \rangle + C_Y^j \langle \hat{P}_k^A \otimes \hat{Y}^B \rangle \\ &+ C_Z^j \langle \hat{P}_k^A \otimes \hat{Z}^B \rangle - C_{-X}^j \langle \hat{P}_k^A \otimes \hat{X}^B \rangle \\ &- C_{-Y}^j \langle \hat{P}_k^A \otimes \hat{Y}^B \rangle - C_{-Z}^j \langle \hat{P}_k^A \otimes \hat{Z}^B \rangle. \end{aligned} \quad (\text{C19})$$

By properties of the a_g , the parameters C_v^j satisfy $0 \leq C_v^j \leq 1$ and $\sum_v C_v^j \leq 1 \forall j$. The normalization is an inequality, as not all a_g will survive Eq. (C15).

For each j , the parameters C_v^j are independent of one another, as they are sums over disjoint sets of the Clifford group. However, for different j values the C_v^j are not guaranteed to be independent of one another, as the separation of the Clifford group into sets defined by the action of its elements on a Pauli operator $\hat{P}_j^B \otimes \hat{I}^{\otimes N_E}$ depends strongly on the specific $\hat{P}_j^B$.

Considering all j gives a total of 18 C_v^j , and we have that $\sum_{j,v} C_v^j \leq 3$. This normalization inequality is saturated when the Clifford-random channel consists of Clifford gates that act nontrivially for all $\hat{P}_j^B \otimes \hat{I}^{\otimes N_E}$, i.e., never take the value of 0 in Eq. (C14).

The second key observation of our derivation is that for the purposes of searching for an optimal attack, we can treat all C_v^j as independent, up to their normalization, as such a search space will necessarily contain all valid C_v^j for a Clifford-random channel attack. Thus, the optimal attack found in this enlarged search space will produce a key rate that is guaranteed to be a lower bound for the worst-case key rate due to a Clifford-random channel attack.

We further assert that *all* valid density matrices in the search space with C_v^j independent correspond to a valid Clifford-random channel attack. We cannot prove that this is the case, but we give a strong argument in what follows. To see that this is likely the case, we contend that there are enough $(N_E + 1)$ -qubit Clifford gates that it is possible to select 18 of them such that $C_v^j = a_{g_v^j}$ are all independent. Other Clifford gates added to the channel can increase the value of one or more C_v^j . In the case where more than one C_v^j have their value increased, then the sum of all C_v^j can exceed unity. This effect, plus the 18 gates giving independent control, is sufficient to generate any value of the free parameters C_v^j such that $0 \leq C_v^j \leq 1$, $\sum_v C_v^j \leq 1 \forall j$, $\sum_{j,v} C_v^j \leq 3$, and $\rho_{AB} \geq 0$. We note that it is possible to select values of C_v^j that do not correspond to a valid Clifford-random attack, but only if one of the constraints listed previously is violated.

The selection of 18 Clifford gates for independent C_v^j implies that each of these gates acts nontrivially [nonzero expectation value in Eq. (C14)] on only one of the three possible initial operators $\hat{P}_j^B \otimes \hat{I}^{\otimes N_E}$. There are three sets of six that each act nontrivially on the same initial operator, and within these sets, each Clifford gate maps the initial Pauli operator to one of the six distinct final Pauli operators (including the ± 1 phase). The selection of 18 such Clifford gates is possible because the elements of the Clifford group realize

all permutations of the Pauli group (with a ± 1 phase) that preserve its commutation structure, and we are considering the $(N_E + 1)$ -qubit Clifford group, with N_E an arbitrarily large, but finite, number.

3. Application to BB84

Consider asymmetric BB84, with the initial state of Alice and Bob given by

$$|\Psi_I\rangle_{AA'} = \sqrt{b}|00\rangle + \sqrt{1-b}|11\rangle, \quad (\text{C20})$$

where $0 \leq b \leq 1$. From this we can work out the expressions for ω_j^k from Eq. (C19). For $\hat{P}_0^A = \mathbb{I}/\sqrt{2}$, $\hat{P}_1^A = \hat{X}/\sqrt{2}$, $\hat{P}_2^A = \hat{Y}/\sqrt{2}$, and $\hat{P}_3^A = \hat{Z}/\sqrt{2}$ we have

$$\omega_j^0 = w_1(C_Z^j - C_{-Z}^j), \quad (\text{C21})$$

$$\omega_j^1 = w_2(C_X^j - C_{-X}^j), \quad (\text{C22})$$

$$\omega_j^2 = -w_2(C_Y^j - C_{-Y}^j), \quad (\text{C23})$$

$$\omega_j^3 = \frac{1}{2}(C_Z^j - C_{-Z}^j), \quad (\text{C24})$$

where

$$w_1 = \frac{1}{2}\langle\Psi_I|_{AA'}\hat{\mathbb{I}}\otimes\hat{Z}|\Psi_I\rangle_{AA'} = \frac{1}{2}(2b-1), \quad (\text{C25})$$

$$\begin{aligned} w_2 &= \frac{1}{2}\langle\Psi_I|_{AA'}\hat{X}\otimes\hat{X}|\Psi_I\rangle_{AA'} \\ &= -\frac{1}{2}\langle\Psi_I|_{AA'}\hat{Y}\otimes\hat{Y}|\Psi_I\rangle_{AA'} = \sqrt{b(1-b)}. \end{aligned} \quad (\text{C26})$$

There is one constraint on Alice's reduced state, given by

$$\omega_0^3 = \frac{1}{2}\langle\Psi_I|_{AA'}\hat{Z}\otimes\hat{\mathbb{I}}|\Psi_I\rangle_{AA'} = w_1. \quad (\text{C27})$$

The full expression for ρ_{AB} is

$$\begin{aligned} \rho_{AB} &= \frac{1}{4}(\mathbb{I} \otimes \mathbb{I} + \omega_0^3 \hat{Z} \otimes \mathbb{I} + \omega_1^0 \hat{\mathbb{I}} \otimes \hat{X} + \omega_2^0 \hat{\mathbb{I}} \otimes \hat{Y} \\ &\quad + \omega_3^0 \hat{\mathbb{I}} \otimes \hat{Z} + \omega_1^1 \hat{X} \otimes \hat{X} + \omega_2^1 \hat{X} \otimes \hat{Y} + \omega_3^1 \hat{X} \otimes \hat{Z} \\ &\quad + \omega_1^2 \hat{Y} \otimes \hat{X} + \omega_2^2 \hat{Y} \otimes \hat{Y} + \omega_3^2 \hat{Y} \otimes \hat{Z} + \omega_1^3 \hat{Z} \otimes \hat{X} \\ &\quad + \omega_2^3 \hat{Z} \otimes \hat{Y} + \omega_3^3 \hat{Z} \otimes \hat{Z}), \end{aligned} \quad (\text{C28})$$

where each ω_j^k contains two free parameters C_μ^j , except for ω_0^3 , which is fixed, as well as the pairs ω_j^0 and ω_j^3 , which both involve C_Z^j . In this calculation we have made no distinction between $\hat{\Omega}_j^k$ and $\hat{\Gamma}_j^k$ and impose the constraints from the known expectation values of the $\hat{\Gamma}_j^k$ as constraints on ρ_{AB} in our convex optimization over the parameters C_μ^j via expressions of the form

$$\text{Tr}[\rho_{AB}\hat{\Gamma}_j^k] = \gamma_j^k. \quad (\text{C29})$$

Note that we have pulled out a factor of $1/2$ from ω_j^k in Eq. (C28).

APPENDIX D: NUMERICAL CALCULATION OF THE SECRET KEY RATE

1. Problem description and dimensional reduction

We follow the general QKD scheme described in [29], using a source replacement scheme to describe the prepare-and-measure protocols under consideration. Alice sends one

half of an initial state $|\Psi_{AB}^I\rangle$ to Bob, and Eve has access to this half of the state before it reaches Bob. Alice and Bob perform measurements on their halves of the final state, described by a set of POVMs, and record the basis they chose to measure in the Hilbert spaces $\bar{A}$ and $\bar{B}$. They record the outcomes of their measurements in Hilbert spaces $\bar{A}$ and $\bar{B}$. For simplicity, we assume that there is a one-to-one mapping of outcomes to key characters, so that the result of the key map is stored in register $\bar{A}$ directly, without the need to introduce another register to store the key-map results (as in the most general protocol described in [29]).

Focusing on the specific example of BB84, the measurement and key-map POVM is described by the operators

$$\begin{aligned} \hat{K}_Z^A &= \sqrt{p}(|0\rangle^{\bar{A}} \otimes \hat{\mathbb{I}}^{\bar{B}} \otimes |0\rangle^{\bar{A}} \otimes \hat{\mathbb{I}}^{\bar{B}} \otimes |0\rangle^A \otimes \hat{\mathbb{I}}^B \\ &\quad + |0\rangle^{\bar{A}} \otimes \hat{\mathbb{I}}^{\bar{B}} \otimes |1\rangle^{\bar{A}} \otimes \hat{\mathbb{I}}^{\bar{B}} \otimes |1\rangle^A \otimes \hat{\mathbb{I}}^B), \end{aligned} \quad (\text{D1})$$

$$\begin{aligned} \hat{K}_X^A &= \sqrt{1-p}(|1\rangle^{\bar{A}} \otimes \hat{\mathbb{I}}^{\bar{B}} \otimes |0\rangle^{\bar{A}} \otimes \hat{\mathbb{I}}^{\bar{B}} \otimes |+\rangle^A \otimes \hat{\mathbb{I}}^B \\ &\quad + |1\rangle^{\bar{A}} \otimes \hat{\mathbb{I}}^{\bar{B}} \otimes |1\rangle^{\bar{A}} \otimes \hat{\mathbb{I}}^{\bar{B}} \otimes |-\rangle^A \otimes \hat{\mathbb{I}}^B), \end{aligned} \quad (\text{D2})$$

$$\begin{aligned} \hat{K}_Z^B &= \sqrt{p}(\hat{\mathbb{I}}^{\bar{A}} \otimes |0\rangle^{\bar{B}} \otimes \hat{\mathbb{I}}^{\bar{A}} \otimes |0\rangle^{\bar{B}} \otimes \hat{\mathbb{I}}^A \otimes |0\rangle^B \\ &\quad + \hat{\mathbb{I}}^{\bar{A}} \otimes |0\rangle^{\bar{B}} \otimes \hat{\mathbb{I}}^{\bar{A}} \otimes |1\rangle^{\bar{B}} \otimes \hat{\mathbb{I}}^A \otimes |1\rangle^B), \end{aligned} \quad (\text{D3})$$

$$\begin{aligned} \hat{K}_X^B &= \sqrt{1-p}(\hat{\mathbb{I}}^{\bar{A}} \otimes |1\rangle^{\bar{B}} \otimes \hat{\mathbb{I}}^{\bar{A}} \otimes |0\rangle^{\bar{B}} \otimes \hat{\mathbb{I}}^A \otimes |+\rangle^B \\ &\quad + \hat{\mathbb{I}}^{\bar{A}} \otimes |1\rangle^{\bar{B}} \otimes \hat{\mathbb{I}}^{\bar{A}} \otimes |1\rangle^{\bar{B}} \otimes \hat{\mathbb{I}}^A \otimes |-\rangle^B), \end{aligned} \quad (\text{D4})$$

with p the probability that Alice (Bob) measures in the Z basis. Note that for $\bar{A}$ we use a key map where the measurement outcome pairs $\{0, +\}$ and $\{1, -\}$ correspond to the same character in the secret key. After these measurements, Alice and Bob will postselect on having measured in the same basis, described by the operator

$$\hat{\Pi} = |0\rangle\langle 0|^{\bar{A}} \otimes |0\rangle\langle 0|^{\bar{B}} \otimes \hat{\mathbb{I}}_4 + |1\rangle\langle 1|^{\bar{A}} \otimes |1\rangle\langle 1|^{\bar{B}} \otimes \hat{\mathbb{I}}_4, \quad (\text{D5})$$

where $\hat{\mathbb{I}}_4$ is a four-qubit identity operator.

The full operation Alice and Bob apply to the state ρ_{AB} is therefore described by the process

$$\begin{aligned} \mathcal{G}(\rho_{AB}) &= \hat{\Pi} \left(\sum_{a,b \in (Z,X)} (\hat{K}_a^A \hat{K}_b^B) \rho_{AB} (\hat{K}_a^A \hat{K}_b^B)^\dagger \right) \hat{\Pi}^\dagger \\ &= (\hat{K}_Z^A \hat{K}_Z^B) \rho_{AB} (\hat{K}_Z^A \hat{K}_Z^B)^\dagger + (\hat{K}_X^A \hat{K}_X^B) \rho_{AB} (\hat{K}_X^A \hat{K}_X^B)^\dagger \\ &= p_z^2 |0\rangle\langle 0|^{\bar{A}} \otimes |0\rangle\langle 0|^{\bar{B}} \otimes \rho_z + p_x^2 |1\rangle\langle 1|^{\bar{A}} \otimes |1\rangle\langle 1|^{\bar{B}} \otimes \rho_x, \end{aligned} \quad (\text{D6})$$

where we have introduced states ρ_z and ρ_x in the $\bar{A}\bar{B}AB$ Hilbert space defined by

$$|0\rangle\langle 0|^{\bar{A}} \otimes |0\rangle\langle 0|^{\bar{B}} \otimes \rho_z = \frac{1}{p_z^2} (\hat{K}_Z^A \hat{K}_Z^B) \rho_{AB} (\hat{K}_Z^A \hat{K}_Z^B)^\dagger, \quad (\text{D7})$$

$$|1\rangle\langle 1|^{\bar{A}} \otimes |1\rangle\langle 1|^{\bar{B}} \otimes \rho_x = \frac{1}{p_x^2} (\hat{K}_X^A \hat{K}_X^B) \rho_{AB} (\hat{K}_X^A \hat{K}_X^B)^\dagger, \quad (\text{D8})$$

with $p_z = p$ and $p_x = 1 - p$ introduced for brevity. We consider a trivial key map from $\bar{A} \rightarrow R$ that copies the values

of register $\bar{A}$ and stores them in register R . As such, we can combine registers $\bar{A}$ and R and act upon $\bar{A}$ as we would upon R for the rest of the calculation [43].

The main numerical task to evaluate the secret key rate is to solve the minimization problem

$$\min_{\rho_{AB}} D(\mathcal{G}(\rho_{AB}) || \mathcal{Z}^{\bar{A}}(\mathcal{G}(\rho_{AB}))), \quad (\text{D9})$$

where, as a reminder, $\mathcal{Z}^{\mathcal{H}}$ is a pinching channel acting on Hilbert space $\mathcal{H}$. In the form currently written, while the minimization is only over $2^2 \times 2^2$ Hermitian matrices, the actual operations themselves involve $2^6 \times 2^6$ size matrices. This is far from ideal in terms of both memory usage and computational time, though not a problem for the original method developed in [29]. However, for the approach used here, the convex approximation to the matrix logarithm creates even larger objects in memory [40], and we have found that the memory usage was far more than what is commonly available on a single work station.

However, we now show that

$$\begin{aligned} D(\mathcal{G}(\rho_{AB}) || \mathcal{Z}^{\bar{A}}(\mathcal{G}(\rho_{AB}))) \\ = p_z^2 D(\rho_{AB} || \mathcal{Z}_Z^A(\rho_{AB})) + p_x^2 D(\rho_{AB} || \mathcal{Z}_X^A(\rho_{AB})), \end{aligned} \quad (\text{D10})$$

where

$$\begin{aligned} \mathcal{Z}_Z^A(\rho_{AB}) &= (|0\rangle\langle 0|^A \otimes \hat{\mathbb{I}}) \rho_{AB} (|0\rangle\langle 0|^A \otimes \hat{\mathbb{I}}) \\ &+ (|1\rangle\langle 1|^A \otimes \hat{\mathbb{I}}) \rho_{AB} (|1\rangle\langle 1|^A \otimes \hat{\mathbb{I}}), \end{aligned} \quad (\text{D11})$$

$$\begin{aligned} \mathcal{Z}_X^A(\rho_{AB}) &= (|+\rangle\langle +|^A \otimes \hat{\mathbb{I}}) \rho_{AB} (|+\rangle\langle +|^A \otimes \hat{\mathbb{I}}) \\ &+ (|-\rangle\langle -|^A \otimes \hat{\mathbb{I}}) \rho_{AB} (|-\rangle\langle -|^A \otimes \hat{\mathbb{I}}), \end{aligned} \quad (\text{D12})$$

with the subscripts of the pinching channels indicating the basis used. Thus, we only need to deal with 4×4 matrices in the optimization, and the secret key rate can be calculated by simultaneous minimization of two relative entropies, with all operations performed in only the AB Hilbert space.

The first step is to prove that

$$\begin{aligned} D(\mathcal{G}(\rho_{AB}) || \mathcal{Z}^{\bar{A}}(\mathcal{G}(\rho_{AB}))) \\ = p_z^2 D(\rho_z || \mathcal{Z}^{\bar{A}}(\rho_z)) + p_x^2 D(\rho_x || \mathcal{Z}^{\bar{A}}(\rho_x)). \end{aligned} \quad (\text{D13})$$

Looking at the structure of Eq. (D6), we see that it can be written in block-diagonal form as

$$\mathcal{G}(\rho_{AB}) = \begin{pmatrix} p_z^2 \rho_z & & & \\ & 0 & & \\ & & 0 & \\ & & & (1-p)^2 \rho_x \end{pmatrix}. \quad (\text{D14})$$

With this in mind, we prove the following lemma to prove Eq. (D13).

Lemma 1. Given two matrices $M = S \oplus T$ and $M' = S' \oplus T'$, where $\dim(S) = \dim(S')$ and $\dim(T) = \dim(T')$, then

$$\text{Tr}[M \log_2(M)] = \text{Tr}[S \log_2(S)] + \text{Tr}[T \log_2(T)], \quad (\text{D15})$$

$$\text{Tr}[M \log_2(M')] = \text{Tr}[S \log_2(S')] + \text{Tr}[T \log_2(T')]. \quad (\text{D16})$$

Using Lemma 1 with the identification $M = \mathcal{G}(\rho_{AB})$ and $M' = \mathcal{Z}^{\bar{A}}(\mathcal{G}(\rho_{AB}))$ proves Eq. (D13). This identification is possible since the pinching channel does not change the block-diagonal structure of $\mathcal{G}(\rho_{AB})$.

We then use the following lemma to prove the full result.

Lemma 2. Given ρ_μ , ρ_{AB} , and $\mathcal{Z}_\mu^{\mathcal{H}}$ defined as before, then

$$D(\rho_z || \mathcal{Z}^{\bar{A}}(\rho_z)) = D(\rho_{AB} || \mathcal{Z}_Z^A(\rho_{AB})), \quad (\text{D17})$$

$$D(\rho_x || \mathcal{Z}^{\bar{A}}(\rho_x)) = D(\rho_{AB} || \mathcal{Z}_X^A(\rho_{AB})). \quad (\text{D18})$$

Equation (D10) follows from application of this lemma to Eq. (D13).

Therefore, solving the minimization problem

$$\min_{\rho_{AB}} p^2 D(\rho_{AB} || \mathcal{Z}_Z^A(\rho_{AB})) + (1-p)^2 D(\rho_{AB} || \mathcal{Z}_X^A(\rho_{AB})) \quad (\text{D19})$$

is equivalent to solving the original minimization problem but only involves the original Hilbert space of Alice and Bob. This considerably reduces the memory and computational power required to numerically calculate the secret key rate. We note that applications of Lemma 1 beyond those discussed here likely exist and that versions of Lemma 2 exist for other QKD protocols [43].

a. Proof of Lemma 1

This result follows straightforwardly from the fact that

$$\log_2(S \oplus T) = \log_2(S) \oplus \log_2(T), \quad (\text{D20})$$

provided that the eigenvalues of S and T fall within the open set $(0, \infty)$. However, the quantum relative entropy is defined on the half-closed set $[0, \infty)$, as we take the convention $0 \times \log_2(0) = 0$. This ensures that $D(\rho || \sigma)$ is finite even when either ρ or σ has eigenvalues that are 0, provided that the support of ρ does not intersect the kernel of σ . Assuming $\text{supp}(\rho) \cap \ker(\sigma) = 0$, our convention ensures that Lemma 1 is valid for $[0, \infty)$ as desired.

b. Proof of Lemma 2

From Eqs. (D7), we have that

$$\rho_z = \hat{L}_Z \rho_{AB} \hat{L}_Z^\dagger, \quad (\text{D21})$$

where

$$\begin{aligned} \hat{L}_Z &= |00\rangle\langle \bar{A}\bar{B}| \otimes |00\rangle\langle 00|^A + |01\rangle\langle \bar{A}\bar{B}| \otimes |01\rangle\langle 01|^A \\ &+ |10\rangle\langle \bar{A}\bar{B}| \otimes |10\rangle\langle 10|^A + |11\rangle\langle \bar{A}\bar{B}| \otimes |11\rangle\langle 11|^A. \end{aligned} \quad (\text{D22})$$

We have that

$$\begin{aligned} &(|0\rangle\langle 0|^{\bar{A}} \otimes \hat{\mathbb{I}}_3) \hat{L}_Z \\ &= |00\rangle\langle \bar{A}\bar{B}| \otimes |00\rangle\langle 00|^A + |01\rangle\langle \bar{A}\bar{B}| \otimes |01\rangle\langle 01|^A \\ &= (\hat{\mathbb{I}}_2 \otimes |0\rangle\langle 0|^A \otimes \hat{\mathbb{I}}) \hat{L}_Z = \hat{L}_Z (\hat{\mathbb{I}}_2 \otimes |0\rangle\langle 0|^A \otimes \hat{\mathbb{I}}) \end{aligned} \quad (\text{D23})$$

and

$$\begin{aligned} & (|1\rangle\langle 1|^{\bar{A}} \otimes \hat{\mathbb{I}}_3) \hat{L}_Z \\ &= |10\rangle^{\bar{A}\bar{B}} \otimes |10\rangle\langle 10|^{AB} + |11\rangle^{\bar{A}\bar{B}} \otimes |11\rangle\langle 11|^{AB} \\ &= (\hat{\mathbb{I}}_2 \otimes |1\rangle\langle 1|^{\bar{A}} \otimes \hat{\mathbb{I}}) \hat{L}_Z = \hat{L}_Z (\hat{\mathbb{I}}_2 \otimes |1\rangle\langle 1|^{\bar{A}} \otimes \hat{\mathbb{I}}), \end{aligned} \quad (\text{D24})$$

and therefore

$$\begin{aligned} \mathcal{Z}^{\bar{A}}(\rho_z) &= \sum_{i=0}^1 (|i\rangle\langle i|^{\bar{A}} \otimes \hat{\mathbb{I}}_3) \hat{L}_Z \rho_{AB} \hat{L}_Z^\dagger (|i\rangle\langle i|^{\bar{A}} \otimes \hat{\mathbb{I}}_3) \\ &= \sum_{i=0}^1 (\hat{\mathbb{I}}_2 \otimes |i\rangle\langle i|^{\bar{A}} \otimes \hat{\mathbb{I}}) \hat{L}_Z \rho_{AB} \hat{L}_Z^\dagger (\hat{\mathbb{I}}_2 \otimes |i\rangle\langle i|^{\bar{A}} \otimes \hat{\mathbb{I}}) \\ &= \mathcal{Z}_Z^A(\rho_z) = \hat{L}_Z (\mathcal{Z}_Z^A(\rho_{AB})) \hat{L}_Z^\dagger. \end{aligned} \quad (\text{D25})$$

Thus, we have reduced the problem to showing that

$$D(\hat{L}_Z \rho_{AB} \hat{L}_Z^\dagger \| \hat{L}_Z (\mathcal{Z}_Z^A(\rho_{AB})) \hat{L}_Z^\dagger) = D(\rho_{AB} \| \mathcal{Z}_Z^A(\rho_{AB})). \quad (\text{D26})$$

Using the fact that

$$L_Z^\dagger L_Z = \hat{\mathbb{I}}_2, \quad (\text{D27})$$

we see that

$$\begin{aligned} & \text{Tr}[\hat{L}_Z \rho_{AB} \hat{L}_Z^\dagger \log_2(\hat{L}_Z \rho_{AB} \hat{L}_Z^\dagger)] \\ &= \text{Tr}[\hat{L}_Z \rho_{AB} \hat{L}_Z^\dagger \hat{L}_Z \log_2(\rho_{AB}) \hat{L}_Z^\dagger] \\ &= \text{Tr}[\rho_{AB} \log_2(\rho_{AB})] \end{aligned} \quad (\text{D28})$$

and

$$\begin{aligned} & \text{Tr}[\hat{L}_Z \rho_{AB} \hat{L}_Z^\dagger \log_2(\hat{L}_Z \mathcal{Z}_Z^A(\rho_{AB}) \hat{L}_Z^\dagger)] \\ &= \text{Tr}[\hat{L}_Z \rho_{AB} \hat{L}_Z^\dagger \hat{L}_Z \log_2(\mathcal{Z}_Z^A(\rho_{AB})) \hat{L}_Z^\dagger] \\ &= \text{Tr}[\rho_{AB} \log_2(\mathcal{Z}_Z^A(\rho_{AB}))], \end{aligned} \quad (\text{D29})$$

which completes the proof for ρ_z . Starting with

$$\rho_x = \hat{L}_X \rho_{AB} \hat{L}_X^\dagger, \quad (\text{D30})$$

$$\begin{aligned} \hat{L}_X &= |00\rangle^{\bar{A}\bar{B}} \otimes |++\rangle\langle ++|^{AB} + |01\rangle^{\bar{A}\bar{B}} \otimes |+-\rangle\langle +-|^{AB} \\ &\quad + |10\rangle^{\bar{A}\bar{B}} \otimes |-+\rangle\langle -+|^{AB} + |11\rangle^{\bar{A}\bar{B}} \otimes |--\rangle\langle --|^{AB} \end{aligned} \quad (\text{D31})$$

and following a procedure similar to that outlined for ρ_z proves the full lemma.

APPENDIX E: HANNEL ESTIMATION AND ERROR CORRECTION

In order to compare the performance of different protocols under these two scenarios, we simulate observed statistics using the depolarizing channel. To put our parametrization of the depolarizing channel in context, for symmetric BB84 ($b = 1/2$), the commonly quoted quantum bit-error rate is half what we define as the depolarizing probability (channel error), ϵ . We use the depolarizing probability rather than the quantum bit-error rate, as for asymmetric protocols there is an inherent bit-error rate even when the channel is perfect ($\epsilon = 0$). For a fair comparison we compare protocols with the same error added by the channel, i.e., the depolarizing probability, rather than the same total error.

As a function of the depolarizing probability the constraints imposed on the SDP by parameter estimation are given by

$$\gamma_{z/x} = \text{Tr}[\mathcal{E}_{\text{dep}}(\rho_{AA'}) \hat{E}_{Z/X}], \quad (\text{E1})$$

$$\gamma_{ij} = \text{Tr}[\mathcal{E}_{\text{dep}}(\rho_{AA'}) \hat{E}_{ij}], \quad (\text{E2})$$

depending on the channel reconciliation protocol chosen. For $b = 1/2$ (i.e., symmetric BB84) the fine-grained constraints reduce to $\gamma_{z/x} = \epsilon/2$ as expected.

From the channel model, we obtain the simulated probability distribution $P(x, y)$ that Alice and Bob would observe from an experiment. In this case, if we assume that the error correction can be performed at the Shannon limit, then $\text{leak}_{\text{EC}} = H(X|Y)$, where X is Alice's raw key and Y is Bob's

measurement outcomes. $H(X|Y)$ is the conditional Shannon entropy,

$$H(X|Y) = - \sum_{x,y} P(x, y) \log_2 P(x|y), \quad (\text{E3})$$

for a joint probability distribution $P(x, y)$ and conditional probability distribution $P(x|y)$. For our purposes, $P(x, y)$ can be calculated via the trace of ρ_{AB} with the appropriate POVM operators for measurement in each basis (see Appendix D for these operators) and is a 4×4 matrix of probabilities. We also incorporate our postselection and sifting into $P(x, y)$, by setting $P(x, y) = 0$ where Alice and Bob did not measure in the same basis (as these events are not used in the key generation), and renormalize $P(x, y)$ by the probability that postselection is successful,

$$p_{\text{pass}} = p^2 + (1 - p)^2, \quad (\text{E4})$$

which is the probability that Alice and Bob both measure in *either* the Z or the X basis. Finally, due to Alice's key map, we add together the elements of $P(x, y)$ for each pair of Alice's raw measurement outcomes that correspond to the same key character, resulting in a 2×4 matrix of probabilities.

APPENDIX F: SECURITY OF THE KEY-RATE LOWER BOUND

The numerical approach used in this work, built off the convex approximation of the quantum relative entropy from Ref. [40], solves an approximate version of the dual problem to obtain a lower bound on the secret key rate. To obtain a *secure* lower bound, one can use the techniques in Ref. [40] to obtain error bounds on the approximation to the quantum relative entropy, in terms of the error bounds on the matrix

FIG. 2. Relative difference between the key-rate lower bound calculated using the convex approximation from Ref. [40] and that using the dual linearization from Ref. [29]. In both cases the unrestricted symmetric ($b = 1/2$) BB84 protocol is considered.

logarithm. Taking the lower bound of these error bounds gives a secure key-rate lower bound. As the order of the approximations used in Ref. [40] is increased, the calculated secret key rate approaches the actual value, and the error bounds become tighter. For all numerical results presented, we have tested increasing orders of approximation, until the value of the key rate was constant up to a threshold value (typically less than 10^{-4}). Thus, we are confident that our numerical results for the key rate lower bound are highly accurate.

As further evidence, for the unrestricted symmetric ($b = 1/2$) BB84 protocol, we have compared the key rate calculated from our approach (using the approximation from Ref. [40]) to that calculated using the dual-linearization approach from [29]. The relative difference between the results of the two approaches is shown in Fig. 2. As can be seen, the key rates are less than a relative difference of 10^{-3} away from one another (i.e., a difference of less than 0.1%). We have not applied the second step method from Ref. [29] to the restricted situation, as this would require deriving a new linearized dual to the SDP of the restricted situation.

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