Second-order coding rates for key distillation in quantum key distribution

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The security of quantum key distribution has traditionally been analyzed in either the asymptotic or non-asymptotic regimes. In this paper, we provide a bridge between these two regimes, by determining second-order coding rates for key distillation in quantum key distribution under collective attacks. Our main result is a formula that characterizes the backoff from the known asymptotic formula for key distillation—our formula incorporates the reliability and security of the protocol, as well as the mutual information variances to the legitimate receiver and the eavesdropper. In order to determine secure key rates against collective attacks, one should perform a joint optimization of the Holevo information and the Holevo information variance to the eavesdropper. We show how to do so by analyzing several examples, including the six-state, BB84, and continuous-variable quantum key distribution protocols (the last involving Gaussian modulation of coherent states along with heterodyne detection). The technical contributions of this paper include one-shot and second-order analyses of private communication over a compound quantum wiretap channel with fixed marginal and key distillation over a compound quantum wiretap source with fixed marginal. We also establish the second-order asymptotics of the smooth max-relative entropy of quantum states acting on a separable Hilbert space, and we derive a formula for the Holevo information variance of a Gaussian ensemble of Gaussian states.

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I. INTRODUCTION

One of the near-term applications of quantum information science is quantum key distribution (QKD) [BB84, Eke91]. By making use of an insecure quantum channel and a public, authenticated classical channel, two parties can share an information-theoretically secure secret key, which can be used later on for one-time pad encryption of a private message. There has been significant progress on this topic in the decades since it was conceived [SBPC+09, Lüt14, LCT14, DLQY16, XMZ+19].

A critical challenge for this research area is to establish security proofs for quantum key distribution. In particular, we are interested in determining the maximum possible rates that are achievable in principle and guaranteed to be secure against any possible eavesdropper allowed by quantum mechanics. Security proofs have been developed for discrete-variable quantum key distribution (DV-QKD) protocols, both in the asymptotic [LC99, SP00, May01, Ko06] and non-asymptotic regimes [Ren05, TLGR12, HT12, TL17]. There are also advanced numerical approaches for addressing the asymptotic security of DV-QKD protocols [CML16, WLC18]. Additionally, security proofs have been developed for continuous-variable quantum key distribution (CV-QKD) protocols [GG02a, GG02b], in the asymptotic [NGA06, GPC06, RC09] and non-asymptotic regimes [FBR+12, Fur14, Lev17]. Furthermore, security proofs have appeared for asymptotic security of discrete-modulation protocols for CV-QKD [ZHRL09, BW18, KGW19, GGD19, LUL19].

In this work, we address the security of quantum key distribution in a regime that represents a bridge between the asymptotic and non-asymptotic regimes. Namely, we employ the methods of second-order asymptotics [Li14, TH13] in order to determine secure key rates for the key distillation step of a quantum key distribution protocol, under the assumption that an adversary applies a collective attack. Our development here covers both DV-QKD and CV-QKD protocols, due to various technical advances that we make in this paper. Second-order quantum information theory grew out of earlier developments in classical information theory [Hay09, PPV10], and it has since been explored extensively for various quantum communication tasks [TT15b, DL15, DTW16, WRG16, TBR16, WTB17, Wil17a, OMW19]. The goal of a second-order information-theoretic analysis is to determine the extra backoff from or overhead on the rates that are achievable in the asymptotic case, which are due to finite-size effects. In the context of quantum key distribution, the approach has been used for analyzing information reconciliation [TTMPE17], for proving upper bounds on secure key rates [WTB17, KW17], and to address the entropy accumulation problem in device-independent QKD [DF19]. See also [Hay06] for earlier work on this topic.

One contribution of our paper is that it is possible to evaluate distinguishable key rates in a regime that goes beyond a first-order asymptotic analysis, which is the typical case studied in several of the aforementioned works [LC99, SP00, May01, Ko06, CML16, WLC18, NGA06, GPC06, RC09, ZHRL09, BW18, KGW19, GGD19, LUL19]. It has been found in several preceding information-theoretic contributions that a second-order analysis gives excellent agreement with what is actually achievable in the finite-size regime [Hay09, PPV10, TBR16, WTB17]. Thus, it is expected that our second-order analysis should agree well with secure distillable key rates that are achievable in principle in the finite-size regime.

To summarize our main contribution to QKD security analysis, suppose that \( \mathcal{S} \) is an “uncertainty set” indexing the states of the eavesdropper Eve that are consistent with the observed measurement results of the sender Alice and the receiver Bob. Let \( p_{XY}(x,y) \) be the probability distribution estimated by Alice and Bob after the parameter estimation step of a QKD protocol [Nota]. For fixed \( s \in \mathcal{S} \), let \( \{p_{XY}(x,y)p_{E|S}^{y,s}(x,y,s)\} \) be an ensemble of states that is consistent with the measurement results of Alice and Bob. Here we are assuming that Eve employs a collective attack, meaning that she applies the same quantum channel to every transmission of Alice.

Then our contribution is that the following is the rate at which secret key bits can be generated in the key distillation step of a direct reconciliation protocol, for sufficiently large \( n \), such that Bob’s decoding error probability is no larger than \( \varepsilon_1 \in (0, 1) \) and the security parameter of the key is no larger than \( \varepsilon_2 \in (0, 1) \):

\[
I(\pi) + \sqrt{\frac{1}{n}V(\pi)}\Phi^{-1}(\varepsilon_1) - \sup_{s \in \mathcal{S}} \left[ I(\pi; E)_s - \frac{1}{n}V(\pi; E)_s\Phi^{-1}(\varepsilon_2^2) \right] + O\left(\frac{\log n}{n}\right),
\]

where

\[
\Phi^{-1}(\varepsilon) := \sup\{a \in \mathbb{R} | \Phi(a) \leq \varepsilon\},
\]

\[
\Phi(a) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{a} dx \exp\left(-\frac{x^2}{2}\right).
\]

In the above, \( I(\pi) \) is the Alice–Bob mutual information, \( V(\pi) \) is the Alice–Bob mutual information variance, \( I(\pi; E)_s \) is the Alice–Eve Holevo information for
fixed $s$, and $V(X; E)_s$ is the Alice–Eve Holevo information variance for fixed $s$. The first-order term is given by 

$$I(X; Y) = \sup_{x \in S} I(X; E)_s,$$

which is the standard information quantity considered in asymptotic security analyses (see, e.g., [Lüt14]). In such a first-order asymptotic analysis, the quantity $I(X; Y) - \sup_{x \in S} I(X; E)_s$ is typically understood as the asymptotic rate at which an imperfect ensemble can be converted to a perfectly secure key. However, this conversion is only perfect in a precise sense in the asymptotic limit. What the mutual information variance $V(X; Y)$ and the Holevo information variance $V(X; E)_s$ characterize are the fluctuations of the first-order terms, which are due to finite-size effects, much like the variance of a random variable characterizes the speed of convergence toward the mean in the central-limit theorem [KS10, She11]. The second-order terms

$$\sqrt{\frac{1}{n} V(X; Y)} \Phi^{-1}(\varepsilon_1)$$

and

$$\sqrt{\frac{1}{n} V(X; E)_s} \Phi^{-1}(\varepsilon^2_1)$$

are negative for $\varepsilon_1, \varepsilon^2_1 < 1/2$, and thus they characterize the back-off from the asymptotic limit for sufficiently large, yet finite $n$. In Section II A 4, we define all of these information quantities formally and explain them in more detail.

For the key distillation step of a reverse reconciliation protocol, the key rate is given by

$$I(X; Y) + \sqrt{\frac{1}{n} V(X; Y)} \Phi^{-1}(\varepsilon_1)$$

$$- \sup_{x \in S} \left[ I(Y; E)_s - \frac{1}{n} V(Y; E)_s \Phi^{-1}(\varepsilon^2_1) \right]$$

$$+ O\left(\frac{\log n}{n}\right). \quad (4)$$

The information quantities appearing in the above formula and their interpretations are essentially the same as those given in (1), with the difference being the substitutions $I(X; E)_s \rightarrow I(Y; E)_s$ and $V(X; E)_s \rightarrow V(Y; E)_s$ to account for reverse reconciliation.

The formulas in (1) and (4) apply regardless of whether the variables $X$ and $Y$ are continuous or discrete, and whether the system $E$ is finite- or infinite-dimensional. It is thus an advantage of our results that the expressions are given in terms of mutual informations and their variances rather than conditional entropies and their variances, as the former ones are well defined for infinite-dimensional systems (see the discussion in [LGG10, Section IV-B]). Furthermore, the above formulas apply whenever $n$ is large enough so that $n \sim \max\{\varepsilon^{-2}_1, \varepsilon^2_1\}$. However, as we stated above, in prior work, this kind of second-order approximation has given excellent agreement with actual finite-size achievability statements [Hay09, PPV10, TBR16, WTB17].

When performing the optimization given by

$$\sup_{x \in S} \left[ I(Y; E)_s - \frac{1}{n} V(Y; E)_s \Phi^{-1}(\varepsilon^2_1) \right], \quad (5)$$

it is possible for large enough $n$ to employ a perturbative approach, in which the first-order term $I(Y; E)_s$ is optimized first, and then among all of the ensembles achieving the optimum first-order term, one further optimizes the second-order term $-\sqrt{\frac{1}{n} V(Y; E)_s} \Phi^{-1}(\varepsilon^2_1)$. See [PPV10, Lemmas 63 and 64] for a justification of this approach.

In Section II, we evaluate achievable secure key rates for three standard QKD protocols: the six-state DV-QKD protocol [Bru98, BPG99], the BB84 DV-QKD protocol [BB84], and the CV-QKD protocol involving Gaussian-modulation coherent-state encodings along with heterodyne detection [GG02a, GG02b]. We find various analytical expressions for the achievable second-order coding rates, and we plot their performance in order to have a sense of what rates are achievable in principle.

We remark here that the contribution of our paper goes beyond the setting of quantum key distribution and applies more broadly in the context of private communication in quantum information theory. A starting point for our development is [Wil17a], but here our result applies more broadly to the scenario in which the Alice–Eve correlations are not precisely known but instead chosen from an “uncertainty set.” Furthermore, our results apply to the scenario in which the underlying quantum states act on an infinite-dimensional, separable Hilbert space (see [HZ12] for a review of this setting of quantum information theory). See Sections III and IV for a one-shot analysis and Section V for a second-order analysis. The information-theoretic setting that we consider here (secure communication against collective attacks) is strongly related to universal private communication and secret key distillation [DH10], as well as the compound wiretap channel and compound wiretap source settings [CCD12, BCCD14, BJ16]. We note here that the compound wiretap setting has been of considerable interest in classical information theory recently [SBP15].

As a side note, it is unclear to us from reading the literature whether researchers working on security analyses against collective attacks in QKD and those working on universal and compound information-theoretic secrecy questions are fully aware of each other, and so one byproduct of our work could be to develop more interaction between these communities. Related to this, the QKD security proof community has been consistently applying the Devetak–Winter formula [DW05] to analyze secret key rates for collective attacks in QKD, in spite of the fact that the Devetak–Winter protocol from [DW05] does not generally apply to such a scenario and instead only applies to a known, fixed attack. The results of our paper also clarify and bridge this gap, and we discuss all of these points in more detail in Section VI.

On a technical level, an important contribution of our paper is to determine the second-order asymptotics of the smooth max-relative entropy (see Appendix F), and this is the main reason why our security analysis applies to the infinite-dimensional case. This result also has impli-
cations for the distinguishing dilution task in the resource theory of asymmetric distinguishability [WW19]. We also extend some other known relations from the finite-to-infinite-dimensional case (see Appendices B, C, D, and E). Combined with the second-order asymptotics of the hypothesis testing relative entropy for the infinite-dimensional case [DPR16, KW17, OMW19], we are then led to our claim concerning second-order coding rates for private communication, secret key distillation, and key distillation in quantum key distribution.

Another technical contribution of our paper is a formula for the Holevo information variance of a Gaussian ensemble of quantum Gaussian states (see Proposition 3 in Appendix H). This formula is useful in a second-order analysis of CV-QKD protocols, and we expect it to be useful in other contexts besides those considered here. We also derive a novel expression for the Holevo information of a Gaussian ensemble of quantum Gaussian states (see Proposition 3).

The rest of the paper proceeds as follows. We first consider the second-order analysis of the key distillation step of quantum key distribution in Section II, and therein we analyze the approach for the important examples mentioned above (six state, BB84, CV-QKD). After that, we then develop the information-theoretic compound wiretap settings and protocols and the corresponding secure rates in detail. In Section VI, we provide a historical discussion of the compound wiretap setting and collective attacks in quantum key distribution, with the stated goal of bridging the communities working on these related topics. We finally conclude in Section VIII with a summary and a list of open questions. The appendices provide details of various technical contributions that are useful for this work and might be of independent interest.

II. SECOND-ORDER CODING RATES FOR KEY DISTILLATION IN QUANTUM KEY DISTRIBUTION

We begin by presenting one of our main results, which is the application of the second-order coding rates in (1) and (4) to the key distillation step of a quantum key distribution protocol. The claim here rests upon the one-shot information-theoretic key distillation protocol from Section IV and its second-order expansion in Section V, the details of which are presented in these later sections. Here we first review a generic prepare-and-measure QKD protocol and then state how (1) and (4) apply in this context. We finally analyze the approach in the context of the six-state DV-QKD protocol [Bru98, BPG99], the BB84 DV-QKD protocol [BB84], and the reverse-reconciliation CV-QKD protocol [GG02b]. All source code files needed to generate the plots in this section are available as ancillary files with the arXiv posting of this paper.

We should clarify that our main emphasis, as indicated above, is on the key distillation step of a quantum key distribution protocol and how to incorporate a second-order coding rate analysis. As part of this, we are assuming that the parameter estimation step of a QKD protocol yields reliable estimates of the classical channel from Alice to Bob that is induced by the quantum part of the QKD protocol. We expand more upon this point in what follows, and we note up front here that it is an open question to incorporate a full second-order analysis that includes the parameter estimation step in addition to the key distillation step.

A. Generic prepare-and-measure QKD protocol

Let us recall the structure of a generic prepare-and-measure protocol for quantum key distribution, in which the adversary applies a collective attack. The protocol consists of three steps: a quantum part, parameter estimation, and key distillation (the last combines information reconciliation and privacy amplification into a single step). We consider both direct and reverse reconciliation settings for key distillation.

1. Quantum part

The quantum part of the protocol consists of the following steps:

1. It begins with the sender Alice picking a state $\rho_A^x$ randomly from an ensemble

$$\mathcal{E}_A := \{p_X(x), \rho_A^x\}_{x \in X},$$

(6)

where $p_X$ is a probability distribution and each state $\rho_A^x$ is described by a density operator acting on an input Hilbert space $\mathcal{H}_A$. 

2. Alice transmits the system $A$ through an unknown quantum channel $\mathcal{N}_{A\to B}$, with input system $A$ and output system $B$. It is assumed that the channel itself is controlled by the eavesdropper Eve, and the output system $B$ is given to the legitimate receiver Bob. It is a standard feature of quantum information that every quantum channel has an isometric extension [Sti55] (see also, e.g., [Wil17b]), from which the original channel can be realized by a partial trace over an environment system. Thus, there exists an isometric channel $\mathcal{U}_{A\to BE}^N$ extending the channel $\mathcal{N}_{A\to B}$ such that

$$\mathcal{N}_{A\to B} = \mathrm{Tr}_E \circ \mathcal{U}_{A\to BE}^N.$$  

(7)

In the worst-case scenario, the eavesdropper has full access to the environment system $E$, and so we assume that she does (as is standard in QKD security proof analyses).

3. Upon receiving the system $B$, the receiver Bob performs a measurement channel $\mathcal{M}_{B\to Y}$, which
is uniquely specified by a positive operator-valued measure (POVM) \( \{ \Lambda_B^y \}_{y \in \mathcal{Y}} \), such that
\[
\Lambda_B^y \geq 0 \quad \forall y \in \mathcal{Y}, \quad \sum_{y \in \mathcal{Y}} \Lambda_B^y = I_B. \tag{8}
\]

According to the Born rule, the measurement channel \( \mathcal{M}_{B \rightarrow Y} \) gives the outcome \( y \) with probability \( \text{Tr}[\Lambda_B^y \omega_B] \) if the input state is \( \omega_B \).

One round of this protocol leads to the following ensemble:
\[
\mathcal{E}_{\text{QKD}} := \mathcal{E}_{\text{QKD}}(\mathcal{E}_A, \mathcal{U}_A^{\mathcal{N}}, \mathcal{M}_{B \rightarrow Y}) := \left\{ (p_{XY}(x, y), \rho_{E}^{x,y} | x \in \mathcal{X}, y \in \mathcal{Y}) \right\}, \tag{9}
\]
where the joint distribution \( p_{XY}(x, y) \) is given as
\[
p_{XY}(x, y) = p_X(x) p_Y(x | y), \tag{11}
\]
\[
p_{Y | X}(y | x) := \text{Tr}[\Lambda_B^y \mathcal{N}_{A \rightarrow B}(\rho_A^x)], \tag{12}
\]
and the eavesdropper states \( \rho_{E}^{x,y} \) are as follows:
\[
\rho_{E}^{x,y} := \frac{\text{Tr}[\Lambda_B^y \mathcal{U}_A^{\mathcal{N}} \mathcal{M}_{B \rightarrow Y} \rho_A^x]}{p_{Y | X}(y | x)}. \tag{13}
\]

Observe how the protocol induces a classical channel \( p_{Y | X}(y | x) \) from Alice to Bob via the Born rule in (12).

The above steps are repeated \( m = k + n \) times, where \( k \) is the number of rounds used for parameter estimation and \( n \) is the number of rounds used for key distillation. The ensemble shared between Alice, Bob, and Eve after these \( m \) rounds is as follows:
\[
\mathcal{E}_{\text{QKD}}^{\otimes m} := \mathcal{E}_{\text{QKD}}^{\otimes m}(\mathcal{E}_A^{\otimes m}, (\mathcal{U}_A^{\mathcal{N}})^{\otimes m}, (\mathcal{M}_{B \rightarrow Y})^{\otimes m}), \tag{14}
\]
\[
:= \left\{ (p_{X^m,Y^m}(x^m, y^m), \rho_{E_{x^m,y^m}}^m) \right\}, x^m \in \mathcal{X}^m, y^m \in \mathcal{Y}^m, \tag{15}
\]
where
\[
p_{X^m,Y^m}(x^m, y^m) := \prod_{i=1}^{m} p_{X,Y}(x_i, y_i), \tag{16}
\]
\[
\rho_{E_{x^m,y^m}}^m := \rho_{E_{x_i,y_i}}^m \otimes \ldots \otimes \rho_{E_{x_1,y_1}}^m, \tag{17}
\]
\[
\rho_{E_{x_i,y_i}}^m := \frac{\text{Tr}[\Lambda_B^y \mathcal{U}_A^{\mathcal{N}} \mathcal{M}_{B \rightarrow Y} \rho_A^x]}{p_{Y \mid X}(y_i| x_i)}, \tag{18}
\]
\[
p_{Y \mid X}(y_i | x_i) := \text{Tr}[\Lambda_B^y \mathcal{N}_{A \rightarrow B} \rho_A^x]. \tag{19}
\]

A critical assumption that we make in the above is that Eve employs a collective attack, meaning that the isometric channel she applies over the \( m \) rounds is the tensor-power channel \( (\mathcal{U}_A^{\mathcal{N}} \mathcal{M}_{B \rightarrow Y})^{\otimes m} \).

\textit{a. Channel twirling} In order to simplify or symmetrize the collective attacks that need to be considered, Alice and Bob can employ an additional symmetrization of the protocol in each round, called channel twirling, introduced in a different context in [BDSW96]. Let \( \{ U_A^g \}_{g \in \mathcal{G}} \) and \( \{ V_B^g \}_{g \in \mathcal{G}} \) be unitary representations of a group \( \mathcal{G} \), such that the unitaries act on the input Hilbert space \( \mathcal{H}_A \) and output Hilbert space \( \mathcal{H}_B \), respectively. Then before sending out her state \( \rho_A^x \), Alice can select \( g \) uniformly at random from the group \( \mathcal{G} \), apply the unitary \( U_A^g \) to her state, communicate the value of \( g \) over a public classical communication channel to Bob, who then performs \( V_B^g \) on his system before acting with his measurement. If Alice and Bob then discard the value of \( g \), this twirling procedure transforms the original quantum channel \( \mathcal{N}_{A \rightarrow B} \) to the following symmetrized quantum channel:
\[
\overline{\mathcal{N}}_{A \rightarrow B}(\omega_A) := \frac{1}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} (V_B^g \circ \mathcal{N}_{A \rightarrow B} \circ U_A^g)(\omega_A), \tag{20}
\]
where
\[
U_A^g(\cdot) := U_A^g(\cdot) U_A^g, \quad V_B^g(\cdot) := V_B^g(\cdot) V_B^g. \tag{21}
\]

Although channel twirling produces a worse (noisier) channel from the original one, the main benefit is that the number of parameters that are needed to specify \( \overline{\mathcal{N}}_{A \rightarrow B} \) can be far fewer than the number needed to specify \( N_{A \rightarrow B} \). For example, if the original channel \( N_{A \rightarrow B} \) is a qubit channel and the unitaries consist of the Pauli operators, then the resulting twirled channel is a Pauli channel and thus specified by only three parameters. If the original channel \( N_{A \rightarrow B} \) is a single-mode bosonic channel and the unitaries consist of the four equally spaced phase rotations \( \{0, \pi/2, \pi, 3\pi/2\} \), then the resulting channel is a phase covariant (phase insensitive) channel [KGW19] and has fewer parameters that characterize it.

\textit{b. Finite-dimensional assumptions} In the trusted device scenario that we are dealing with here, if the Hilbert space \( \mathcal{H}_A \) is finite dimensional, then we are making an implicit assumption that the union of the supports of the states \( \rho_A^x \) are fully contained in the Hilbert space \( \mathcal{H}_A \) and there is no leakage outside of it. In the case that system \( B \) is finite dimensional (i.e., the Hilbert space \( \mathcal{H}_B \) is finite dimensional), then we are making an implicit assumption that the measurement operators \( \{ \Lambda_B^y \}_{y \in \mathcal{Y}} \) satisfy \( \sum_{y \in \mathcal{Y}} \Lambda_B^y = I_B \) and that \( I_B \) is indeed the identity operator for \( \mathcal{H}_B \). Thus, if both the input and output Hilbert spaces \( \mathcal{H}_A \) and \( \mathcal{H}_B \) are finite dimensional, then by the Choi–Kraus theorem (see, e.g., [Wil17b]), it is not necessary for Eve’s system to be any larger than \( \text{dim}(\mathcal{H}_A) \cdot \text{dim}(\mathcal{H}_B) \). So it follows that the finite dimensional assumption leads to strong constraints about Eve’s attack, which may not necessarily hold in practice and thus should be stated up front. This is especially the case when dealing with photonic states and measurements acting on subspaces of an infinite-dimensional bosonic Fock space.

2. \textit{Sifting} Some QKD protocols, such as the six-state and BB84 protocols, incorporate a sifting step, in which a fraction
of the data generated by the protocol is discarded. The main reason for incorporating sifting is that some input-output pairs in \( X \times Y \) do not give any useful information about the channel (Eve’s attack) and thus can be discarded. For example, if the input state is \(|0\rangle|0\rangle\) or \(|1\rangle|1\rangle\) and Bob measures in the basis \([+]|+, |−⟩|−\rangle\), then even in the noiseless case of no eavesdropping, the outcome of the measurement is independent of the input and thus yields no useful information.

This sifting step can be described mathematically as a filter onto a subset \( F \subseteq X \times Y \), with the sifting probability given by

\[
p_{\text{sift}} := \sum_{(x,y) \in F} p_{XY}(x,y),
\]

and the conditioned ensemble by

\[
\mathcal{E}_{\text{QKD}}^{\text{sift}} := \left\{ p'_{XY}(x,y), p'_{E|x} \right\}_{(x,y) \in F},
\]

where

\[
p'_{XY}(x,y) := p_{XY}(x,y)/p_{\text{sift}}.
\]

As a consequence of sifting, some number \( m' \) of the original \( m \) rounds are selected, and the remaining systems of Alice, Bob, and Eve are described by the tensor-power ensemble:

\[
(\mathcal{E}_{\text{QKD}}^{\text{sift}})^{\otimes m'} := \left\{ p'_{X^{m'}Y^{m'}}, p'_{E^{m'}|x'Y^{m'}} \right\}_{(x',y') \in F^{m'}},
\]

with the above quantities defined similarly as in (14)–(19).

In the discussion that follows in Section II A 3, we simply relabel \( m' \) as \( m \) and the distribution \( p'_{XY}(x,y) \) as \( p_{XY}(x,y) \), with it understood that elements of \( p_{XY}(x,y) \) with \( (x,y) \) outside of \( F \) are set to zero. The distribution \( p_X \) is the marginal of \( p_{XY} \), and the conditional distribution \( p_{Y|X} \) is a classical channel computed from \( p_{XY} \) as usual via \( p_{XY}(x,y)/p_X(x) \).

3. Parameter estimation

After \( m \) rounds of the protocol are complete, \( k \) of the XY classical systems are randomly selected by Alice and Bob for parameter estimation, in order to estimate the set \( S \) of possible collective attacks of Eve. To be clear, the classical systems used for parameter estimation are \( X_{i_1}, Y_{i_1}, \ldots, X_{i_k}, Y_{i_k} \) for some randomly selected (without replacement) \( i_1, \ldots, i_k \in \{1, \ldots, n\} \).

In what follows, we assume that \( k \) is large enough such that Alice and Bob get a very reliable (essentially exact) estimate of the classical channel \( p_{Y|X}(y|x) \). This assumption is strong, but as stated above, our main focus in this paper is on analyzing second-order coding rates in the key distillation step of the quantum key distribution protocol. In Section II C, we discuss various routes for addressing this problem.

The goal of the parameter estimation step is to estimate the classical channel \( p_{Y|X}(y|x) \) reliably in order to produce an estimate of the unknown quantum channel \( N_{A\rightarrow B} \) connecting Alice and Bob. Doing so then allows them to estimate the isometric channel \( U_{A\rightarrow BE'} \) up to an information theoretically irrelevant isometry acting on the system \( E \). In more detail, note that any other isometric extension of the original channel \( N_{A\rightarrow B} \) is related to \( U_{A\rightarrow BE'} \) by an isometric channel acting on the system \( E \). That is, suppose that \( V'_{A\rightarrow BE'} \) is another isometric channel satisfying \( N_{A\rightarrow B} = V'_{A\rightarrow BE'} \). Then there exists an isometric channel \( W_{E\rightarrow E'} \) such that \( V'_{A\rightarrow BE'} = W_{E\rightarrow E'} \circ U_{A\rightarrow BE'} \) [Wil17]. However, Eve’s information about the classical systems \( X \) and \( Y \) is the same regardless of which particular isometric extension is considered. Thus, as stated above, the goal of the parameter estimation step is to estimate the channel \( N_{A\rightarrow B} \) by employing the estimate of \( p_{Y|X}(y|x) \).

As a result of the parameter estimation step, Alice and Bob determine an uncertainty set \( S \), each element \( s \) of which indexes a quantum channel \( N_{A\rightarrow B} \) that is consistent with the classical channel \( p_{Y|X}(y|x) \), in the sense that

\[
p_{Y|X}(y|x) = \text{Tr}[\Lambda^s_{B'}N_{A\rightarrow B}^s(\rho_A^s)],
\]

for all \( s \in S, x \in X \), and \( y \in Y \). It is generally not possible to determine the actual quantum channel \( N_{A\rightarrow B} \) exactly, so that \(|S| > 1 \). However, if the input ensemble \( E_A = \{ p_X(x), \rho_A^s \}_x \in X \) and the POVM \( \{ \Lambda^s_B \}_y \in Y \) form a tomographically complete set [CN97, PCZ97], then it is possible to determine an exact estimate of the actual, unknown quantum channel \( N_{A\rightarrow B} \) from the classical channel \( p_{Y|X}(y|x) \). That is, in the tomographically complete case, there exists an invertible linear map relating \( p_{Y|X}(y|x) \) and \( N_{A\rightarrow B} \). So in this special case, there is a unique quantum channel \( N_{A\rightarrow B} \) corresponding to the classical channel \( p_{Y|X}(y|x) \).

In some parameter estimation protocols, Alice and Bob do not estimate the entries of \( p_{Y|X}(y|x) \) for all \( x \in X \) and \( y \in Y \) (for example as a consequence of sifting). Furthermore, they could reduce the number of parameters that need to be estimated by employing additional symmetrization of \( p_{Y|X}(y|x) \), in which some of the entries are averaged or simple functions of them are computed. These latter approaches are commonly employed in the parameter estimation phase of the BB84 and six-state protocols, in which quantum bit error rates (QBERs) are estimated in lieu of all entries of \( p_{Y|X}(y|x) \). Another example for which the full \( p_{Y|X}(y|x) \) is not typically estimated is CV-QKD, where only two scalar parameters are estimated in order to derive a key-rate lower bound under a collective-attack assumption, even in a finite key-length regime [Lev15].
4. Key distillation

After the parameter estimation step, the ensemble characterizing each of the $n$ remaining systems shared by Alice, Bob, and Eve is as follows:

$$E_{\text{QKD}}^n := \left\{ p_{XY}(x,y), \rho_{E}^{x,y,s} \right\}_{x \in X, y \in Y, s \in S},$$

(27)

where

$$p_{XY}(x,y) = p_X(x)p_{Y|X}(y|x),$$

(28)

$$p_{Y|X}(y|x) := \text{Tr} \left[ \Lambda_B^y \Lambda_A^s \right],$$

(29)

and the eavesdropper states $\rho_{E}^{x,y,s}$ are as follows:

$$\rho_{E}^{x,y,s} := \frac{\text{Tr}_B \left[ \Lambda_B^y \Lambda_A^s \rho_A^s \right]}{p_{Y|X}(y|x)}.$$  

(30)

The full ensemble for the $n$ remaining systems is an $n$-fold tensor power of the above, similar to that given in (14)–(19), except with the substitutions $m \rightarrow n$ and $\mathcal{N}^s \rightarrow \mathcal{N}^s$. Note that the classical channel $p_{Y|X}(y|x)$ is known and independent of $s$, due to our assumption of a collective attack and that $k$ is large enough so that Alice and Bob can estimate $p_{Y|X}(y|x)$ reliably. That is, there could be many quantum channels $\mathcal{N}^s$ that lead to the same classical channel $p_{Y|X}(y|x)$ if the input preparation and the output measurements are not tomographically complete. Furthermore, the distribution $p_X(x)$ is known because Alice controls the random selection of the states $\{\rho_A^s\}_{x \in X}$.

The ensemble in (27) is then a particular instance of the information-theoretic model presented later on in Section IV. Specifically, the ensemble in (27) is an instance of the composite wiretap source with fixed marginal from (211), in which the system $B$ in (211) is in correspondence with the classical system $Y$ in (27). As a result, we can apply (251) (itself a consequence of Theorem 6) to conclude that the following rate is achievable for key distillation for the remaining $n$ rounds, by using direct reconciliation:

$$I(X;Y)_{\mathcal{E}} := \sum_{x \in X, y \in Y} p_{XY}(x,y) \log_2 \left( \frac{p_{XY}(x,y)}{p_X(x)p_Y(y)} \right),$$

(32)

the classical mutual information variance as [Str62, Hay09, PPV10]

$$V(X;Y)_{\mathcal{E}} := \sum_{x \in X, y \in Y} p_{XY}(x,y) \left[ \log_2 \left( \frac{p_{XY}(x,y)}{p_X(x)p_Y(y)} \right) - I(X;Y)_{\mathcal{E}} \right]^2,$$

(33)

the Holevo information as [Hol73]

$$I(X;E)_{\mathcal{E}} := \sum_{x \in X} p_X(x) D(\rho_{E}^{x,s} \| \rho_{E}^s),$$

(34)

and the Holevo information variance as

$$V(X;E)_{\mathcal{E}} := \sum_{x \in X} p_X(x) \left[ V(\rho_{E}^{x,s} \| \rho_{E}^s) + [D(\rho_{E}^{x,s} \| \rho_{E}^s)]^2 \right] - [I(X;E)_{\mathcal{E}}]^2,$$

(35)

where

$$\rho_{E}^{x,s} := \sum_{y \in Y} p_{Y|X}(y|x) \rho_{E}^{x,y,s},$$

(36)

$$\rho_{E}^s := \sum_{x \in X} p_X(x) \rho_{E}^{x,s}.$$  

(37)

The quantum relative entropy of states $\omega$ and $\tau$ is defined as [Ume62]

$$D(\omega \| \tau) := \text{Tr} \left[ \omega \left( \log_2 \omega - \log_2 \tau \right) \right],$$

(38)

and the quantum relative entropy variance as [Li14, TH13]

$$V(\omega \| \tau) := \text{Tr} \left[ \omega \left( \log_2 \omega - \log_2 \tau \right)^2 \right].$$

(39)

These quantities are defined more generally in (248)–(249) for states acting on separable Hilbert spaces. If either alphabet $X$ or $Y$ is continuous, then the corresponding sum is replaced with an integral.

If Alice and Bob employ reverse reconciliation instead for key distillation, then the following distillable key rate is achievable:

$$I(X;Y)_{\mathcal{E}} + \sqrt{\frac{1}{n} V(X;Y)_{\mathcal{E}} \Phi^{-1}(\epsilon_1)}$$

$$- \sup_{s \in S} \left[ I(Y;E)_{\mathcal{E}} - \sqrt{\frac{1}{n} V(Y;E)_{\mathcal{E}} \Phi^{-1}(\epsilon_1)} \right] + O \left( \frac{\log n}{n} \right),$$

(40)
with the Holevo information defined as
\[ I(Y; E)_{\varepsilon^*} := \sum_{y \in Y} p_Y(y)D(\rho^y_{e} || \rho^*_{e}), \tag{41} \]
and the Holevo information variance as
\[ V(Y; E)_{\varepsilon^*} := \sum_{y \in Y} p_Y(y) \left[ V(\rho^y_{e} || \rho^*_{e}) + [D(\rho^y_{e} || \rho^*_{e})]^2 \right] - [I(Y; E)_{\varepsilon^*}]^2, \tag{42} \]
where
\[ \rho^y_{e} := \sum_{x \in X} p_{X|Y}(x|y)\rho^y_{e|x}. \tag{43} \]

Remark 1: We emphasize that the formulas in (31) and (40) represent the number of secret key bits per sifted bit. If we include all of the rounds of the protocol as part of the key rate, then the formulas in (31) and (40) must be multiplied by the fraction of bits used for sifting; see, e.g., [TL17, Eq. (121)].

a. On reconciliation efficiency and privacy amplification overhead. It is common in the key distillation step of a first-order asymptotic analysis to incorporate a reconciliation efficiency parameter \( \beta \in [0, 1] \), which recognizes the fact that it is never possible in any realistic scheme to achieve the Shannon limit \( I(X; Y)_{\varepsilon^*} \). That is, the information reconciliation rate is written as \( \beta I(X; Y)_{\varepsilon^*} \).

Typically, the reconciliation efficiency \( \beta \) is chosen as a constant independent of the channel, the blocklength \( n \), and the decoding error probability \( \varepsilon_1 \). As argued in [TMMPE17], this approximation is rather rough, and one can instead employ a second-order analysis to get a much better approximation of the reconciliation efficiency. What we find from (31) and (40) is that the ideal reconciliation efficiency is characterized in terms of \( p_{XY} \), \( n \), and \( \varepsilon_1 \) as follows:
\[ \beta(p_{XY}, n, \varepsilon_1) := 1 + \sqrt{\frac{1}{n} V(X; Y)_{\varepsilon^*} \Phi^{-1}(\varepsilon_1)} \frac{\Phi^{-1}(\varepsilon_1)}{I(X; Y)_{\varepsilon^*}}, \tag{44} \]
so that
\[ \beta(p_{XY}, n, \varepsilon_1) I(X; Y)_{\varepsilon^*} = I(X; Y)_{\varepsilon^*} + \sqrt{\frac{1}{n} V(X; Y)_{\varepsilon^*} \Phi^{-1}(\varepsilon_1)}. \tag{45} \]
(Keep in mind that \( \Phi^{-1}(\varepsilon_1) < 0 \) for \( \varepsilon_1 < 1/2 \).) One can also find very good fits of the information reconciliation performance for actual codes by allowing for constants \( \beta_1 \) and \( \beta_2 \), each not necessarily equal to one, to characterize the reconciliation efficiency empirically as follows [TMMPE17]:
\[ \beta(p_{XY}, n, \varepsilon_1, \beta_1, \beta_2) := \beta_1 + \beta_2 \sqrt{\frac{1}{n} V(X; Y)_{\varepsilon^*} \Phi^{-1}(\varepsilon_1)} \frac{\Phi^{-1}(\varepsilon_1)}{I(X; Y)_{\varepsilon^*}}, \tag{46} \]
Thus, the formula above is a more useful guideline for reconciliation efficiency.

What we also notice in (31) and (40) is the presence of terms related to privacy amplification overhead. Privacy amplification overhead beyond the term \( \sup_{s \in S} I(Y; E)_{\varepsilon^*} \) is not typically taken into account in first-order asymptotic security analyses, in spite of the fact that other factors are inevitably necessary. To be clear, the privacy amplification overhead is a factor \( \gamma > 1 \) that multiplies the asymptotic, first-order term \( \sup_{s \in S} I(Y; E)_{\varepsilon^*} \). By employing [PPV10, Lemma 63], the following expansion in \( n \) holds for direct-reconciliation privacy amplification for sufficiently large \( n \):
\[ \sup_{s \in S} I(Y; E)_{\varepsilon^*} = -\sqrt{\frac{1}{n} V(X, S^*) \Phi^{-1}(\varepsilon^2_1)} + o(1/\sqrt{n}), \tag{47} \]
where
\[ V(X, S^*) := \begin{cases} \sup_{s \in S} V(X; E)_{\varepsilon^*} & \text{if } \varepsilon^2_1 \leq \frac{1}{2} \varepsilon_1, \\ \inf_{s \in S} V(X; E)_{\varepsilon^*} & \text{else} \end{cases}, \tag{48} \]
\[ S^* := \arg \max_{s \in S} I(X; E)_{\varepsilon^*}. \tag{49} \]
In the above, we are applying the perturbative approach of [PPV10, Lemma 63], in which we optimize the first-order term \( I(X; E)_{\varepsilon^*} \), and then among all of the optimizers of this first-order term, we are optimizing the second-order term \( V(X; E)_{\varepsilon^*} \). Thus, the ideal privacy amplification overhead is given by
\[ \gamma(S, n, \varepsilon_1) := 1 - \frac{1}{\sup_{s \in S} I(X; E)_{\varepsilon^*}} \frac{V(X, S) \Phi^{-1}(\varepsilon^2_1)}{I(X; E)_{\varepsilon^*}}, \tag{50} \]
so that
\[ \gamma(S, n, \varepsilon_1) \sup_{s \in S} I(X; E)_{\varepsilon^*} = \sup_{s \in S} I(X; E)_{\varepsilon^*} - \sqrt{\frac{1}{n} V(X, S^*) \Phi^{-1}(\varepsilon^2_1)}. \tag{51} \]
As above, we could also allow for a more refined expression as follows, in terms of constants \( \gamma_1 \) and \( \gamma_2 \), in order to fit the performance of realistic privacy amplification protocols:
\[ \gamma(S, n, \varepsilon_1, \gamma_1, \gamma_2) := \gamma_1 - \gamma_2 \sqrt{\frac{1}{n} V(X, S^*) \Phi^{-1}(\varepsilon^2_1)} \sup_{s \in S} I(X; E)_{\varepsilon^*}. \tag{52} \]

B. Examples

1. General setup for the six-state and BB84 DV-QKD protocols

We begin this example section by providing the general setup for both the ideal, trusted six-state [Bru98, BPG99]
and BB84 [BB84] DV-QKD protocols, which are particular instances of the generic prepare-and-measure protocol presented in Section II A.

In both of these protocols, the random variable $X$ for Alice’s encoding is a joint random variable consisting of random variables $X_1$ and $X_2$, where $X_1$ represents Alice’s basis choice, and $X_2$ is the binary random variable corresponding to the state taken from the chosen basis. The random variables $X_1$ and $X_2$ are independent. We similarly have that the output random variable $Y$ for Bob is a joint random variable consisting of random variables $Y_1$ and $Y_2$, where $Y_1$ represents the choice of measurement basis, and $Y_2$ represents the outcome of the measurement.

Let the alphabet $B$ contain the possible basis choices. The random variables $X_1$ and $Y_1$ take values in $B$. For the six-state protocol, $B_{six-state} = \{0, 1, 2\}$, with “0” denoting the $X$-basis, “1” the $Z$-basis, and “2” the $Y$-basis. For the BB84 protocol, $B_{BB84} = \{0, 1\}$. Then, let $q_A^b$ and $q_B^b$ be the probabilities that Alice and Bob, respectively, choose the basis $b \in B$. In other words,\

$$q_A^b := \Pr[X_1 = b], \quad q_B^b := \Pr[Y_1 = b].$$  \hfill (53)

Let us define the following:

$$
\begin{align*}
\Pi_0^b &\equiv |+\rangle\langle +| = \rho_A^{00}, \\
\Pi_1^b &\equiv |-\rangle\langle -| = \rho_A^{01}, \\
\Pi_2^b &\equiv |0\rangle\langle 0| = \rho_A^{10}, \\
\Pi_3^b &\equiv |1\rangle\langle 1| = \rho_A^{11}, \\
\Pi_4^b &\equiv |+i\rangle\langle +i| = \rho_A^{20}, \\
\Pi_5^b &\equiv |-i\rangle\langle -i| = \rho_A^{21},
\end{align*}
$$  \hfill (54)

where\

$$
\begin{align*}
|+\rangle &\equiv (|0\rangle + |1\rangle)/\sqrt{2}, \\
|-\rangle &\equiv (|0\rangle - |1\rangle)/\sqrt{2}, \\
|+i\rangle &\equiv (|0\rangle + i|1\rangle)/\sqrt{2}, \\
|-i\rangle &\equiv (|0\rangle - i|1\rangle)/\sqrt{2}.
\end{align*}
$$  \hfill (55)

Now, Alice chooses the basis $b \in B$ with probability $q_A^b$, and with probability $1/2$ chooses one of the two states $\{\rho_A^{00}, \rho_A^{11}\}$ in the basis to send to Bob. These choices are independent, and so we have that\

$$p_{X_1X_2}(b_A, x) = q_A^b \cdot \frac{1}{2}. \hfill (64)$$

The encoding ensemble $E_A$ is thus\

$$E_A := \{p_{X_1X_2}(b_A, x), \rho_A^{b_Ax}\}_{b_A \in B, x \in \{0,1\}}. \hfill (65)$$

The decoding POVM for Bob is\

$$P_{b_B}^{b_b} := \{q_B^b \Pi_B^{b_y}\}_{b_B \in B, y \in \{0,1\}}, \hfill (66)$$

which is equivalent to Bob picking the basis $b_B$ at random according to $q_B^b$ and then performing the measurement $\{\Pi_B^{b_y}\}$. The protocol is finite dimensional, meaning that the assumptions stated in Section II A 1b, come into play. Thus, the attack $\mathcal{N}_{A-B}$ that Eve applies is a qubit channel.

The channel twirling that Alice and Bob perform in this case is a Pauli channel twirl [BDSW96]. That is, before sending out her state, Alice applies, uniformly at random, one of the Pauli operators $I$, $X$, $Y$, or $Z$ and Bob applies the corresponding Pauli after receiving the state from the channel. Thus, both $\{U^g_A\}_{g \in G}$ and $\{V^g_B\}_{g \in G}$, as discussed in Section II A 1a, are the Pauli group $\{I, X, Y, Z\}$. Then the resulting twirled channel is as given in (20), and it is well known that a Pauli twirl of a qubit channel leads to a Pauli channel [DHCB05]:\

$$\mathcal{N}_{A-B}(\omega_A) = p_I \omega_A + p_X X \omega_A X + p_Y Y \omega_A Y + p_Z Z \omega_A Z,$$  \hfill (67)

where $p_I, p_X, p_Y, p_Z \geq 0$ and $p_I + p_X + p_Y + p_Z = 1$.

Note that it is not necessary for Alice and Bob to apply the Pauli channel twirl in an active way in the quantum domain. Since the encoding ensemble in (65) is invariant with respect to the Pauli group (for both the six-state and BB84 protocols), Alice can keep track of the twirl in classical processing. Similarly, the decoding POVM of Bob in (66) is invariant with respect to the Pauli group, so that Bob can keep track of the twirl in classical processing.

At the end of the quantum part of the protocol, the induced classical channel is as follows:

$$p_{Y_1Y_2|X_1X_2}(b_B, y|b_A, x) = q_B^b \frac{1}{\text{Tr}[\Pi_B^{b_y} \mathcal{N}_{A-B}(\rho_A^{b_Ax})]]}. \hfill (68)$$

The joint probability distribution shared by Alice and Bob is then as follows:

$$p_{X_1X_2Y_1Y_2}(b_A, x, b_B, y) = p_{Y_1Y_2|X_1X_2}(b_B, y|b_A, x)p_{X_1X_2}(b_A, x) \hfill (69)$$

$$= \frac{1}{2} q_A^b q_B^b \frac{1}{\text{Tr}[\Pi_B^{b_y} \mathcal{N}_{A-B}(\rho_A^{b_Ax})]} \hfill (70)$$

Both the six-state and BB84 protocols involve a sifting step, as discussed in Section II A 2. Only the data are kept for which the sender and receiver’s basis bits agree. The probability that Alice and Bob choose the same basis is given by:

$$p_{sift} := \sum_{b \in B} q_A^b q_B^b \hfill (71)$$

The resulting probability distribution shared by Alice and Bob is:

$$p_{X_1X_2Y_1Y_2}^{sift}(x, b, y) := \frac{q_A^b q_B^b}{p_{sift}} \frac{1}{\text{Tr}[\Pi_B^{b_y} \mathcal{N}_{A-B}(\rho_A^{b_Ax})]], \hfill (72)$$

and it is for this (conditional) probability distribution that parameter estimation occurs and using which key distillation occurs in both the six-state and BB84 protocols.
The full classical-classical-quantum state of Alice, Bob, and the eavesdropper, can be written via an isometric extension \( \mathcal{U}_{A \rightarrow BE} \) of the channel \( \mathcal{N}_{A \rightarrow B} \). Specifically,

\[
\rho_{X_1X_2Y_1Y_2E}^{\text{sift}} = \sum_{b \in B} \sum_{x,y=0}^1 \frac{q_b^A q_b^B}{p_{\text{sift}}} p_{X_2Y_2|X_1Y_1}^{b}(x,y|b,b) |b,b\rangle\langle b,b|_{X_1Y_1} \otimes |x,y\rangle\langle x,y|_{X_2Y_2} \otimes \rho_E^{b,x,y},
\]

where

\[
p_{X_2Y_2|X_1Y_1}^{b}(x,y|b,b) = \frac{1}{2} \text{Tr}_i[\Pi_y^{E} \mathcal{N}_{A \rightarrow B}(\rho_A^{b})],
\]

and

\[
\rho_E^{b,x,y} = \frac{\text{Tr}_B[\Pi_y^{E} \mathcal{U}_{A \rightarrow BE}(\rho_A^{b,x})]}{p_{X_2Y_2|X_1Y_1}^{b}(x,y|b,b)}. \tag{75}
\]

The channel parameters \( p_X, p_Y, \) and \( p_Z \) in (67) can be rewritten in terms of three quantum bit error rates (QBERs) \( Q_x, Q_y, \) and \( Q_z \), which in each case corresponds to the expected probability that Bob measures a different state from what Alice sent with respect to a given basis:

\[
Q_x := \frac{1}{2} \left( (|0\rangle\langle 0| + |1\rangle\langle 1|)/\sqrt{2} \right),
\]

\[
Q_y := \frac{1}{2} \left( (|+\rangle\langle +| - |\rangle\langle -|)/\sqrt{2} \right),
\]

\[
Q_z := \frac{1}{2} \left( (|\rangle\langle 0| + |\rangle\langle 1|)/\sqrt{2} \right).
\]

The probabilities \( p_X, p_Y, \) and \( p_Z \) are then related to \( Q_x, Q_y, \) and \( Q_z \) as follows:

\[
p_X = \frac{1}{2} (Q_x - Q_z + Q_y), \tag{79}
\]

\[
p_Y = \frac{1}{2} (Q_x - Q_y + Q_z), \tag{80}
\]

\[
p_Z = \frac{1}{2} (Q_y - Q_z + Q_x). \tag{81}
\]

See [Kha16, Chapter 2] for a derivation of these equations. In the six-state protocol, it is possible to estimate all of the QBERs reliably, while in BB84, it is only possible to estimate \( Q_x \) and \( Q_z \) reliably.

Another further symmetrization of the protocol, in addition to channel twirling, is possible if Alice and Bob discard the basis information in \( X_1 \) and \( Y_1 \). This is commonly employed in both the six-state and BB84 protocols in order to simplify their analysis. Discarding the basis information corresponds to tracing out the registers \( X_1 \) and \( Y_1 \) containing the basis information for Alice and Bob, respectively:

\[
\rho_{X_2Y_2E}^{\text{sift}} := \text{Tr}_{X_1Y_1}[\rho_{X_1X_2Y_1Y_2E}^{\text{sift}}] = \sum_{x,y=0}^1 \frac{q_b^A q_b^B}{p_{\text{sift}}} p_{X_2Y_2|X_1Y_1}^{b}(x,y|b,b) |x,y\rangle\langle x,y|_{X_2Y_2} \otimes \rho_E^{b,x,y}. \tag{82}
\]

This discarding of basis information in either the six-state or BB84 protocols is equivalent to a further channel twirl. Let us consider first the six-state protocol, and let \( T \) denote the following unitary

\[
T := |+\rangle\langle 0| - |\rangle\langle -| = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -i \\ 1 & i \end{bmatrix}, \tag{83}
\]

so that \( T \) is a unitary changing the Pauli basis as

\[
TXT^\dagger = Y, \tag{84}
\]

\[
TYT^\dagger = Z, \tag{85}
\]

\[
TZT^\dagger = X. \tag{86}
\]

Due to the fact that this gate swaps information encoded into the Pauli eigenstates around, discarding of basis information in the six-state protocol is equivalent to a further channel twirl as [Myh10, Section 2.2.7]

\[
\mathcal{N}_{A \rightarrow B}^Q(\omega_A) := \frac{1}{3} \sum_{j \in \{0,1,2\}} T_j^{1/2} \mathcal{N}_{A \rightarrow B}(T_j \omega_A T_j)^{1/2} \tag{87}
\]

\[
= \left( 1 - \frac{3Q}{2} \right) \omega_A + \frac{Q}{2} \left( X \omega_A X + Y \omega_A Y + Z \omega_A Z \right), \tag{88}
\]

where

\[
Q = \frac{1}{3} (Q_x + Q_y + Q_z). \tag{89}
\]

The channel \( \mathcal{N}_{A \rightarrow B}^Q \) above is the well known quantum depolarizing channel. It is completely positive for \( Q \in [0,2/3] \), and it is entanglement breaking when \( Q \in [1/3,2/3] \). An entanglement breaking channel is not capable of distilling secret key, as argued in [CLL04], with a strong limitation for the finite-key regime established in [WTB17].

Now let us consider the BB84 protocol. Let \( H \) denote the following unitary Hadamard transformation:

\[
H := |+\rangle\langle 0| + |\rangle\langle -| = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \tag{90}
\]

so that \( H \) changes the Pauli \( X \) and \( Z \) bases as \( HXH^\dagger = Z \) and \( HZH^\dagger = X \). Due to the fact that the \( H \) gate swaps information encoded into the Pauli \( X \) and \( Z \) eigenstates around, discarding of basis information in the BB84 protocol is equivalent to a further channel twirl as [Myh10, Section 2.2.7]

\[
\mathcal{N}_{A \rightarrow B}^{BB84,Q}(\omega_A) := \frac{1}{2} \sum_{j \in \{0,1\}} H_j^{1/2} \mathcal{N}_{A \rightarrow B}(H_j^{1/2} \omega_A H_j^{1/2}) H_j^{1/2} \tag{91}
\]

\[
= (1 - 2Q + s) \omega_A + (Q - s) X \omega_A X.
\]
where in this case
\[ Q = \frac{1}{2} (Q_x + Q_z), \quad (93) \]
\[ s = Q - Q_y/2. \quad (94) \]

The channel \( N_{A\to B}^{BB84,Q} \) is thus known as the BB84 channel in the literature [SS08]. Observe that \( s \in [2Q - 1, Q] \) in order for complete positivity to hold. By computing the Choi state of this channel and using the condition for separability from [ADH08], we find that the BB84 channel is entanglement breaking for \( s \in [0, 1/2] \) and \( Q \in [(s + 1/2)/2, (s + 1)/2] \). As before, it is not possible to distill secret key from the BB84 channel when it is entanglement breaking.

We call a protocol in which the basis information is discarded a “coarse-grained protocol”. We find analytic expressions for the key distillation rate of the coarse-grained BB84 and six-state protocols in the following sections.

2. Six-state protocol

For the six-state protocol, we have \( B = B_{\text{six-state}} = \{0, 1, 2\} \), corresponding to the \( X, Y, Z \) bases. We typically take \( q^b_A = \frac{1}{3} = q^b_B \) for all \( b \in B \), so that \( p_{\text{sift}} = \frac{1}{3} \). The joint distribution shared by Alice and Bob after sift is as follows:

\[
6\text{-state|sift}\:
\begin{align*}
p_{X_1X_2Y_1Y_2}(b, x, b, y) &= \frac{q^A_B q^B_A}{2p_{\text{sift}}} \text{Tr}[\rho^y_{A|B}(\rho^b_A|x)],
\end{align*}
\]

for \( b \in \{0, 1, 2\} \) and \( x, y \in \{0, 1\} \). Each of the relevant entries is given by

\[
\begin{align*}
p_{X_1X_2Y_1Y_2}(0, 0, 0, 0) &= \frac{1}{6}(1 - Q_x), \quad (96) \\
p_{X_1X_2Y_1Y_2}(0, 0, 0, 1) &= \frac{1}{6}Q_x, \quad (97) \\
p_{X_1X_2Y_1Y_2}(0, 0, 1, 0) &= \frac{1}{6}Q_x, \quad (98) \\
p_{X_1X_2Y_1Y_2}(0, 1, 0, 0) &= \frac{1}{6}(1 - Q_x), \quad (99) \\
p_{X_1X_2Y_1Y_2}(1, 0, 0, 0) &= \frac{1}{6}(1 - Q_z), \quad (100) \\
p_{X_1X_2Y_1Y_2}(1, 0, 1, 0) &= \frac{1}{6}Q_z, \quad (101) \\
p_{X_1X_2Y_1Y_2}(0, 1, 1, 0) &= \frac{1}{6}Q_z, \quad (102) \\
p_{X_1X_2Y_1Y_2}(1, 1, 1, 0) &= \frac{1}{6}(1 - Q_z), \quad (103) \\
p_{X_1X_2Y_1Y_2}(1, 1, 1, 1) &= \frac{1}{6}(1 - Q_z), \quad (104) \\
p_{X_1X_2Y_1Y_2}(2, 0, 2, 0) &= \frac{1}{6}(1 - Q_y), \quad (105) \\
p_{X_1X_2Y_1Y_2}(2, 0, 2, 1) &= \frac{1}{6}Q_y, \quad (106) \\
p_{X_1X_2Y_1Y_2}(2, 1, 2, 0) &= \frac{1}{6}Q_y, \quad (107) \\
p_{X_1X_2Y_1Y_2}(2, 1, 2, 1) &= \frac{1}{6}(1 - Q_y). \quad (108)
\end{align*}
\]

Let us define the average QBER as

\[ Q := \frac{1}{3}(Q_x + Q_y + Q_z). \quad (109) \]

If Alice and Bob discard the basis information in \( X_1 \) and \( Y_1 \), then the resulting probability distribution is

\[
\begin{align*}
p_{X_2Y_2}(0, 0) &= \frac{1}{2}(1 - Q), \quad (109) \\
p_{X_2Y_2}(0, 1) &= \frac{1}{2}Q, \quad (110) \\
p_{X_2Y_2}(1, 0) &= \frac{1}{2}Q, \quad (111) \\
p_{X_2Y_2}(1, 1) &= \frac{1}{2}(1 - Q). \quad (112)
\end{align*}
\]

In other words, when discarding the basis information, Alice and Bob’s data can be characterized by the single parameter \( Q \).

For the six-state protocol, there is a reliable estimate of Eve’s collective attack. This means that the uncertainty set \( S \) discussed in Section II A 3 has cardinality equal to one. With the further assumption of discarding basis information, the average QBER \( Q \) uniquely identifies the attack of Eve, as in (88). By following the derivations in Appendix A, we find that the mutual and Holevo informations and variances as a function of the average QBER \( Q \) are as follows:

\[
\begin{align*}
I(X; Y)_\rho &= 1 - h_2(Q), \quad (113) \\
V(X; Y)_\rho &= Q(1 - Q) \left( \log_2 \left( \frac{1 - Q}{Q} \right) \right)^2, \quad (114) \\
I(X; E)_\rho &= -\left( 1 - \frac{3Q}{2} \right) \log_2 \left( 1 - \frac{3Q}{2} \right) \right) - h_2(Q), \quad (115) \\
V(X; E)_\rho &= Q + \left( 1 - \frac{3Q}{2} \right) \left( \log_2 \left( \frac{1 - 3Q}{1 - Q} \right) \right)^2 \right) \right) + \frac{1}{2} \left( \log_2 \left( \frac{Q}{1 - Q} \right) \right)^2 - I(X; E)_\rho^2, \quad (116)
\end{align*}
\]

where

\[ h_2(Q) := -Q \log_2(Q) - (1 - Q) \log_2(1 - Q) \quad (117) \]

is the binary entropy. The achievable distillable key with direct reconciliation is then given by evaluating the general formula in (31):

\[
K_{6\text{-state}}(Q, \varepsilon_1, \varepsilon_{11}) = 1 + \left( 1 - \frac{3Q}{2} \right) \log_2 \left( 1 - \frac{3Q}{2} \right)
\]
The probability distribution is equal to the known asymptotic key rate for the six-state protocol after sifting with $Q = 0.05$. The purple solid line indicates the asymptotic key rate.

$$\begin{align*}
    &+ \frac{3Q}{2} \log_2 \left( \frac{Q}{2} \right) \\
    &+ \sqrt{Q(1-Q)} \log_2 \left( \frac{1-Q}{Q} \right) \Phi^{-1}(\varepsilon_1) \\
    &+ \sqrt{\frac{V(X; E)_p}{n}} \Phi^{-1}(\varepsilon_{11}^2). 
\end{align*}$$

(118)

We note that the first-order rate term in the above expression is equal to the known asymptotic key rate for the six-state protocol and coincides with the result from [AMKB11].

Figure 1 plots the second-order coding rate for key distillation using the six-state protocol. These rates can be compared with the finite-key analysis from [AMKB11], but the comparison is not necessarily fair, due to our assumption of reliable parameter estimation.

We finally note that incorporating the methods of [KR08] can improve the key rate.

3. **BB84 DV-QKD protocol**

For the BB84 protocol, we have $\mathcal{B} = \mathcal{E}_{BB84} = \{0, 1\}$, corresponding to the $X$ and $Z$ bases. We typically take $\theta_b = \frac{1}{2} = \theta_A$ for all $b \in \mathcal{B}$, so that $p_{\text{sift}} = \frac{1}{2}$. The relevant probability distribution is

$$p_{X,b,sift}(b, x, y) = \frac{q_b^A q_b^B}{2p_{\text{sift}}} \text{Tr}[\hat{N}_{A \rightarrow B}(\rho_A^{b,x})],$$

(119)

for $b \in \{0, 1\}$ and $x, y \in \{0, 1\}$. We then have

$$p_{X,b,sift}(0,0,0,0) = \frac{1}{4}(1-Q_x),$$

(120)

$$p_{X,b,sift}(0,0,0,1) = \frac{1}{4}Q_x,$$

(121)

$$p_{X,b,sift}(0,1,0,0) = \frac{1}{4}(1-Q_z),$$

(122)

$$p_{X,b,sift}(0,1,0,1) = \frac{1}{4}Q_z,$$

(123)

$$p_{X,b,sift}(1,0,0,0) = \frac{1}{4}(1-Q_z),$$

(124)

$$p_{X,b,sift}(1,0,0,1) = \frac{1}{4}Q_z,$$

(125)

$$p_{X,b,sift}(1,1,0,0) = \frac{1}{4}(1-Q_z),$$

(126)

$$p_{X,b,sift}(1,1,0,1) = \frac{1}{4}Q_z,$$

(127)

Let us define the average QBER as

$$Q := \frac{1}{2}(Q_x + Q_z).$$

(128)

If Alice and Bob discard the basis information in $X_1$ and $Y_1$, then the probability distribution is

$$p_{X,b,sift}(0,0) = \frac{1}{2}(1-Q),$$

(129)

$$p_{X,b,sift}(0,1) = \frac{1}{2}Q,$$

(130)

$$p_{X,b,sift}(1,0) = \frac{1}{2}Q,$$

(131)

$$p_{X,b,sift}(1,1) = \frac{1}{2}(1-Q).$$

(132)

In other words, when discarding the basis information, Alice and Bob’s classical data can be characterized using the single parameter $Q$.

For the parameter estimation step of the protocol, it is possible for Alice and Bob to determine the QBERs $Q_x$ and $Q_z$ reliably. However, it is not possible to estimate $Q_y$ because the encoding and decoding do not involve the eigenbasis of the Pauli $Y$ operator. Thus, the uncertainty set $\mathcal{S}$ in this case consists of all Pauli channels satisfying (79)–(81) for fixed $Q_x$ and $Q_z$. If we further simplify the protocol by throwing away the basis information, then the analysis simplifies. By following the derivations in Appendix $A$, we find that the mutual and Holevo informations and variances as a function of the average QBER $Q$ and the optimization parameter $s \in [0, Q]$ are as follows:

$$I(X; Y)_p = 1 - h_2(Q),$$

(133)

$$V(X; Y)_p = Q(1-Q) \left( \log_2 \left( \frac{1-Q}{Q} \right) \right)^2,$$

(134)

$$I(X; E)_p = H(\{1-2Q+s, Q-Q+s, Q-s, s\}) - h_2(Q),$$

(135)

$$V(X; E)_p = (1-2Q+s) \left( \log_2 \left( \frac{1-2Q+s}{1-Q} \right) \right)^2 + (Q-s) \left( \log_2 \left( \frac{Q-s}{1-Q} \right) \right)^2,$$

(136)
The achievable key rate for direct reconciliation is then given by evaluating the general formula in (31) and performing an optimization over the parameter \( s \in [0, Q] \). We note that the first-order rate term \( I(X; Y) - I(X; E) \) is equal to the known asymptotic key rate for the BB84 protocol and coincides with the result from [SP00].

Figure 2 plots the second-order coding rate for key distillation using the BB84 protocol. These rates can be compared with the finite-key analysis from [TL17], but the comparison is not necessarily fair, due to our assumption of reliable parameter estimation.

We again note that incorporating the methods of [SRS08] can improve the key rate.

4. CV-QKD protocol with coherent states and heterodyne detection

We finally analyze the performance of the CV-QKD Gaussian modulation protocol with reverse reconciliation. This protocol involves Gaussian modulation of coherent states by Alice and heterodyne detection by Bob, and it is a particular instance of the prepare-and-measure protocol from Section II A.

The encoding ensemble \( \mathcal{E}_A \) in this case is

\[
\{p_{\pi}(\alpha), |\alpha\rangle\langle\alpha| \}_{\alpha \in \mathbb{C}}, \tag{137}
\]

where \( \pi > 0 \), \( p_{\pi}(\alpha) \) is an isotropic complex Gaussian distribution:

\[
p_{\pi}(\alpha) := \frac{1}{\pi \pi} \exp \left( -|\alpha|^2 / \pi \right), \tag{138}
\]

and \(|\alpha\rangle\langle\alpha|\) is a coherent state [GK04] such that

\[
|\alpha\rangle := e^{-|\alpha|^2 / 2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle, \tag{139}
\]

with \( \{|n\rangle\}_{n=0}^{\infty} \) the orthonormal photon number basis. The decoding POVM for Bob is heterodyne detection [GK04], given by

\[
\left\{ \frac{1}{\pi} |\alpha\rangle\langle\alpha| \right\}_{\alpha \in \mathbb{C}}. \tag{140}
\]

Let \( X \) be a complex random variable corresponding to the choice of \( \alpha \) in Alice’s encoding, and let \( Y \) be a complex random variable corresponding to Bob’s measurement outcome.

The encoding and decoding act on a single bosonic mode, which implies that the channel \( \mathcal{N}_{A\rightarrow B} \) that Eve employs is a single-mode bosonic channel.

The channel twirling that Alice and Bob employ in this case is the phase symmetrization from [KGW19]. In particular, before Alice sends out a coherent state, she applies the unitary \( e^{-i \phi} \), with the phase \( \phi \) selected uniformly at random from \( \{0, \pi/2, \pi, 3\pi/2\} \). She communicates this choice to Bob, who then applies \( e^{i \alpha \phi} \) to his received mode. They both then discard the classical memory of which phase \( \phi \) was applied. This phase symmetrization significantly reduces the number of parameters that Alice and Bob need to estimate in the parameter estimation part of the protocol. Like the other protocols, this phase symmetrization need not be applied in the quantum domain because the encoding ensemble in (137) and the decoding POVM (140) are invariant under the actions of Alice and Bob mentioned above. Thus, it can be carried out in classical processing that keeps track of the twirl.

During the parameter estimation step of the protocol, Alice and Bob estimate

\[
\gamma_{12} := E\{(X - E\{X\})^* (Y - E\{Y\})\}, \tag{141}
\]

\[
\gamma_{22} := E\{|Y - E\{Y\}|^2\}. \tag{142}
\]

We suppose here that the photon number variance of the channel output system \( B \) is finite, in order to ensure that reliable estimation of the parameters \( \gamma_{12} \) and \( \gamma_{22} \) is possible. Here we also assume that they estimate \( p_{Y|X}(y|x) \). The following parameter is known

\[
\gamma_{11} := E\{|X - E\{X\}|^2\}, \tag{143}
\]

being a function of Alice’s encoding ensemble. The uncertainty set \( S \) in this case then consists of all single-mode bosonic channels, with system \( B \) having finite photon number variance, that lead to the estimates \( \gamma_{12} \) and \( \gamma_{22} \), as well as \( p_{Y|X}(y|x) \). The achievable key rate is given by evaluating the formula in (40) as a function of the encoding in (137), the decoding in (140), and the set \( S \) mentioned above. To evaluate this formula, we apply the perturbative approach from [PPV10, Lemmas 63 and 64].
which is valid for sufficiently large $n$. In this approach, we optimize the first-order Holevo information term of Eve first, and then among all of the channels optimizing the first-order term, we optimize the second-order Holevo information variance of Eve. In this case, the Gaussian extremality theorem of [WGC06], as observed in [GPC06], implies that a Gaussian attack achieves the optimal first-order Holevo information of Eve. The same conclusion has been reached in [NGA06] by a different line of reasoning. In fact, by examining the proof in [NGA06] employing the faithfulness of quantum relative entanglement, we just evaluate it with respect to the optimal and unique Gaussian attack.

We stress here that, even though the actual attack of Eve need not be a Gaussian channel, the Gaussian optimality theorem and the perturbative extension of it is useful in order to bound Eve’s information from above. Without this result, the optimization would be too difficult (perhaps impossible) because the underlying Hilbert space is infinite-dimensional.

Let us analyze the performance of the above protocol in a particular physical scenario. Suppose that the underlying physical channel is indeed a thermal channel \( L^{n,N_B}_{A\rightarrow B} \) [Ser17], characterized by transmissivity \( \eta \in (0,1) \) and environmental thermal photon number \( N_B \). However, Alice and Bob are not aware of this, as is the usual case in a QKD protocol. They execute the above protocol, and after the parameter estimation step, suppose that they have estimated the classical channel \( p_{Y|X}(y|x) \) and the parameters in (141)–(142). From the parameters in (141)–(142), they conclude that the optimal Gaussian attack of Eve is a thermal channel of transmissivity \( \eta \) and environment thermal photon number \( N_B \). Let \( U^{n,N_B}_{A\rightarrow B,E} \) be an isometric channel extending \( L^{n,N_B}_{A\rightarrow B} \). An isometric channel extending \( L^{n,N_B}_{A\rightarrow B} \) can be physically realized by the action of a beamsplitter of transmissivity \( \eta \) acting on the input mode \( A \) and one share \( E_1 \) of a two-mode squeezed vacuum state \( \psi^{n}_E \) as in (144),

\[
\psi^{n}_E := |\psi_{E_1}^{N_B}|_{E_1E_2} := \frac{1}{\sqrt{N_B+1}} \sum_{n=0}^{\infty} \left( \frac{\sqrt{N_B}}{N_B+1} \right)^n |n\rangle_E_1 |n\rangle_E_2.
\]

We now calculate the various quantities in (40) for this case and for a reverse reconciliation protocol. We begin by determining the mutual information \( I(X;Y) \) and the mutual information variance \( V(X;Y) \). The classical channel \( p_{Y|X}(y|x) \) induces by heterodyne detection of a Gaussian-distributed ensemble of coherent states transmitted through the thermal channel \( L^{n,N_B}_{A\rightarrow B} \) is as follows (see, e.g., [Guh04, Sav12]):

\[
p_{Y|X}(y|x) = \exp \left( -\frac{|y-\sqrt{\eta}x|^2}{\pi ((1-\eta)N_B+1)} \right),
\]

where \( x, y \in \mathbb{C} \). As mentioned previously, we assume that this classical channel \( p_{Y|X} \) is reliably estimated during the parameter estimation step [Notb]. Then it follows that

\[
I(X;Y) = \log_2 (1 + P),
\]

\[
V(X;Y) = \frac{1}{\ln^2 2} \frac{P(P+2)}{(P+1)^2},
\]

where

\[
P := \frac{\eta \bar{n}}{(1-\eta)N_B+1}.
\]

The formulas above follow from the fact that the channel \( p_{Y|X}(y|x) \) in (146) can be understood as two independent real Gaussian channels each with signal-to-noise ratio \( P \), and then by applying Shannon’s formula [Sha48] and the mutual information variance formula from [PPV10, TT15a] with a prefactor of two to account for the two independent channels. We now turn to calculating the Holevo information \( I(Y;E) \) and the Holevo information variance \( V(Y;E) \), the latter of which can be calculated as a special case of Proposition 3 below. For a Gaussian-distributed ensemble of coherent states as in (138), the expected input density operator is a thermal state of the following form [Ser17]:

\[
\theta(\bar{n}) := \frac{1}{\bar{n}+1} \sum_{n=0}^{\infty} \left( \frac{\bar{n}}{\bar{n}+1} \right)^n |n\rangle\langle n|,
\]

with covariance matrix \( V(\bar{n}) := (2\bar{n} + 1)I_2 \), where \( I_2 \) is the \( 2 \times 2 \) identity matrix. It then follows that the covariance matrix of the state \( \rho_{BE} := U^{n,N_B}_{A\rightarrow B,E}(\theta(\bar{n})) \) is

\[
V_{\rho_{BE}} := \begin{bmatrix} V_B & V_{BE} \\ V_{BE} & V_E \end{bmatrix} = \begin{bmatrix} B(\eta) \oplus I_2 \end{bmatrix} V(\bar{n}) V(E(N_B)) \begin{bmatrix} B^T(\eta) \oplus I_2 \end{bmatrix},
\]
where
\[
B(\eta) := \begin{bmatrix} \sqrt{\eta} I_2 & \sqrt{1-\eta} I_2 \\ -\sqrt{1-\eta} I_2 & \sqrt{\eta} I_2 \end{bmatrix},
\]
(153)
\[
V_E(N_B) := \begin{bmatrix} (2N_B + 1) I_2 & 2\sqrt{N_B(N_B + 1)} \sigma_Z \\ 2\sqrt{N_B(N_B + 1)} \sigma_Z & (2N_B + 1) I_2 \end{bmatrix}.
\]
(154)

For this example, note that Eve’s actual attack and Alice and Bob’s estimation of it coincide, due to our assumption that the underlying channel is a thermal channel. We then obtain the covariance matrix of the reduced state \(\rho_E = \text{Tr}_B[\rho_{BE}]\) from the above, which can be used to calculate the entropy \(H(E)\). The covariance matrix of the reduced state \(\rho_Z^E\) of Eve’s system, given the outcome \(y\) of Bob’s heterodyne detection is as follows:

\[
V_{E|Y} := V_E - V_{BE} (V_B + I_2)^{-1} V_{BE}^T,
\]
(155)
and the probability of obtaining the outcome \(y\) is

\[
p_Y(y) := \frac{\exp\left(-\frac{|y|^2}{\pi(\eta \eta + (1 - \eta) N_B + 1)}\right)}{\eta \eta + (1 - \eta) N_B + 1}.
\]
(156)

This allows us to compute the conditional entropy as

\[
H(E|Y) = \int dy \ p_Y(y) H(E)\rho_E.
\]
(157)

Now combining \(H(E)\rho_E - H(E|Y) = I(Y; E),\) we can calculate Eve’s Holevo information.

To calculate the Holevo information variance \(V(Y; E),\) we apply the formula from Proposition 3 below. To understand this formula, we first provide a definition for a Gaussian ensemble of quantum Gaussian states.

**Definition 2 (Gaussian ensemble)** A Gaussian ensemble of \(m\)-mode Gaussian states consists of a Gaussian prior probability distribution of the form

\[
p_Y(y) := \mathcal{N}(\mu, \Sigma)
\]
(158)
\[
:= \frac{\exp\left(-\frac{1}{2}(y - \mu)^T \Sigma^{-1} (y - \mu)\right)}{\sqrt{(2\pi)^{2m} \det(\Sigma)}},
\]
(159)
and a set \(\{\rho_E^y\}_{y \in \mathbb{R}^{2n}}\) of Gaussian states, each having \(2m \times 1\) mean vector \(W y + \nu\) and \(2m \times 2m\) quantum covariance matrix \(V.\) In the above, \(y\) is a \(2n \times 1\) vector, \(\mu\) is the \(2n \times 1\) mean vector of the random vector \(Y,\) \(\Sigma\) is the \(2n \times 2n\) covariance matrix of the random vector \(Y,\) \(W\) is a \(2m \times 2n\) matrix, and \(\nu\) is a \(2m\)-dimensional vector.

**Proposition 3** The Holevo information of the ensemble in Definition 2 is given by

\[
I(Y; E) = \frac{1}{2 \ln^2 2} \left[ \ln \left( \frac{Z_E}{Z} \right) + \frac{1}{2} \text{Tr}[V \Delta] + \text{Tr}[W \Sigma W^T G_E]\right],
\]
(160)

See Appendix H for a review of quantum Gaussian states and measurements and for a proof of Proposition 3.

Putting everything above together, we find that the achievable secret key rate is given by evaluating the above quantities in the formula in (40). Figure 3 plots the second-order coding rate for key distillation using the CV-QKD reverse reconciliation protocol. One can compare these rates to the finite-key analysis presented in [Lev15], but the comparison is not necessarily fair due to our assumption of reliable parameter estimation. We also note that the first-order term in (40) is equal to the known asymptotic key rate from [Lev15].

![FIG. 3. Distillable key rates for the reverse reconciliation CV-QKD protocol, when conducted over a thermal channel with transmissivity \(\eta = 0.2\) and environment photon number \(N_B = 10^{-2}\). The purple solid line indicates the asymptotic key rate.](image-url)
C. Routes to a full second-order analysis that includes parameter estimation

As we have mentioned in Section II A 3, our second-order analysis above is incomplete, in the sense that it does not incorporate details of the parameter estimation step. That is, we have assumed that $k$ is large enough to allow for a reliable estimate of the induced classical channel $p_{Y|X}$, and from there, we applied a second-order analysis to the key distillation step. Here we discuss a potential route around this issue and an avenue for future work on this topic.

For finite-dimensional protocols, the collective attack of Eve is constrained to a finite-dimensional quantum channel. This quantum channel is realized by a unitary acting on a larger, yet finite-dimensional Hilbert space. If we limit Eve to a finite set of quantum computations that could be realized from a finite, universal gate set, which could in principle realize any unitary on the space to any desired accuracy, then the resulting channel is selected from a very large, yet finite and known set. In this case, the parameter estimation procedure of [Pol13, Sec-III-D] can be applied, and it has negligible overhead. Indeed, it is possible to estimate the channel chosen from a finite set with $k = O(\log n)$ and such that the decoding error probability is increased by no more than $1/\sqrt{n}$, which has no impact on the second-order terms in (31) and (40) for sufficiently large $n$. However, the main drawback of this approach is that, even though this constraint on the eavesdropper might be considered reasonable, it is still a computational assumption and thus lies outside the quantum information-theoretic security that is ultimately desired in quantum key distribution. Furthermore, this does not address CV-QKD protocols in which there is not a finite-dimensional assumption.

Another approach to address the issue is to incorporate recent advances in universal coding up to the second order [Hay19]. A universal code does not depend on the particular channel over which communication is being conducted, and it only requires an estimate of the first- and second-order terms. This approach has been analyzed in detail in [Hay19], and it is likely that it could be combined with the information-theoretic protocol considered in this paper and the parameter estimation step in order to arrive at a full second-order analysis for both the parameter estimation and key distillation steps in a quantum key distribution protocol. A benefit of this approach is that quantum information-theoretic security would be retained. We leave a full investigation of this approach for future work.

III. PRIVATE COMMUNICATION OVER A COMPOUND WIREDATA CHANNEL WITH FIXED MARGINAL

We now present the one-shot information-theoretic results that underlie the previous claims for key distillation in quantum key distribution. We begin by considering private communication over a compound wiretap channel with fixed marginal, and then in Section IV, we move on to a key distillation protocol for a compound wiretap source with fixed marginal.

A. One-shot setting

In the setting of private communication, we suppose that Alice, Bob, and Eve are connected by means of the following classical–quantum–quantum (cqq) compound wiretap channel with fixed marginal:

$$\mathcal{N}_{X \rightarrow BE}^s : x \rightarrow \rho_{BE}^{x,s},$$  \hspace{1cm} (168)

where the classical input $x \in \mathcal{X}$, the alphabet $\mathcal{X}$ is countable, the index $s \in \mathcal{S}$ represents the choice or state of the channel, the set $\mathcal{S}$ can be uncountable, and $\rho_{BE}^{x,s}$ is a density operator acting on the tensor-product separable Hilbert space $\mathcal{H}_B \otimes \mathcal{H}_E$. We suppose that the channel has a fixed marginal; i.e., the reduced Alice-Bob channel

$$\mathcal{N}_{X \rightarrow B}^s : x \rightarrow \rho_B^{x,s} := \text{Tr}_E[\rho_{BE}^{x,s}]$$  \hspace{1cm} (169)

is known to Alice and Bob, so that

$$\rho_B^{x,s} = \rho_B^s \quad \text{for all} \quad s \in \mathcal{S}. \hspace{1cm} (170)$$

However, the reduced $s$-dependent Alice-Eve channel

$$\mathcal{N}_{X \rightarrow E}^s : x \rightarrow \rho_E^{x,s} := \text{Tr}_B[\rho_{BE}^{x,s}]$$  \hspace{1cm} (171)

is not fully known to or characterized by Alice or Bob during their communication. Thus, the channel $\mathcal{N}_{X \rightarrow BE}$ is a particular member of a set $\mathcal{S}$ of channels, for which

$$\text{Tr}_E[\rho_{BE}^{x,s}] = \rho_B^s \quad \text{for all} \quad s \in \mathcal{S}. \hspace{1cm} (172)$$

To be clear, we suppose that the set $\mathcal{S}$ is known to Alice and Bob, but the particular channel indexed by $s \in \mathcal{S}$, which is actually being employed during the communication protocol, is not known. The goal of a private communication protocol is for Alice to send a message securely to Bob, such that it is secure against the channel $\mathcal{N}_{X \rightarrow BE}$ for all $s \in \mathcal{S}$.

The action of the channel in (168) can be described in the fully quantum picture as follows:

$$\mathcal{N}_{X \rightarrow BE}(\omega_X) := \sum_x (|x\rangle_X \omega_X |x\rangle_X \rho_{BE}^{x,s}),$$  \hspace{1cm} (173)

where $\{|x\rangle_X\}_{x \in \mathcal{X}}$ is a countable orthonormal basis for an input separable Hilbert space $\mathcal{H}_X$.

In our model of communication, we suppose also that public shared randomness is available for free to Alice and Bob. Since it is public, Eve gets a copy of all of the shared randomness. In particular, therefore, this shared randomness is not the same as prior secret key shared by Alice and Bob.
Let \( \Psi_{RA RB RE} \) denote the following public shared randomness state:
\[
\Psi_{RA RB RE} := \sum_{r=1}^{\lvert A \rvert} p(r) |r \rangle \langle r |_{RA} \otimes |r \rangle \langle r |_{RB} \otimes |r \rangle \langle r |_{RE},
\]
where \( R \) is the alphabet for the shared randomness, Alice possesses the classical register \( RA \), Bob \( RB \), and Eve \( RE \). The systems \( RA, RB, \) and \( RE \) have the same dimension.

A private coding scheme for the channel in (168) consists of the public shared randomness state \( \Psi_{RA RB RE} \), an encoding channel \( E_{RA M} \to X \) taking the register \( RA \) and a message register \( M \) to the channel input register \( X \), and a decoding channel \( D_{RB \to M} \). Two parameters \( \varepsilon_1 \) and \( \varepsilon_{II} \) determine the decoding error probability and the security of the protocol, respectively. Alice uses the coding scheme and the channel in (168) to send a message \( m \in \mathcal{M} \), where \( \mathcal{M} \) is the message alphabet, and the conditional probability of decoding as \( m' \in \mathcal{M} \) is given by
\[
\Pr[\hat{M} = m' | M = m] := \langle m' | \hat{M} D_{RB \to M}(\rho_{BRB}^m) | m \rangle_{\hat{M}},
\]
where
\[
\rho_{BRB}^m := \text{Tr}_{ER}[\rho_{BERB RE}^m],
\]
\[
\rho_{BERB RE}^m := (\mathcal{N}^s_{X \to BE} \otimes E_{RA M} \to X)(|m \rangle \langle m |_M \otimes \Psi_{RA RB RE}).
\]

Note that the reduced state \( \rho_{BRB}^m \) has no dependence on \( s \), due to the assumption stated in (172). To see (175) in a different way, we can alternatively consider Bob's positive operator-valued measure \( \{\Lambda^m_{RB} \}_{m \in \mathcal{M}} \) to consist of the following elements:
\[
\Lambda^m_{RB} := (D_{RB \to M})^\dagger (|m \rangle \langle m |_M),
\]
where \( (D_{RB \to M})^\dagger \) is the Hilbert–Schmidt adjoint of the decoding channel \( D_{RB \to M} \), so that we can write \( \Pr[\hat{M} = m' | M = m] \) in terms of the Born rule as
\[
\Pr[\hat{M} = m' | M = m] = \text{Tr}[\Lambda^m_{RB} \rho_{BRB}^m].
\]

The protocol is \( \varepsilon_1 \)-reliable, with \( \varepsilon_1 \in [0, 1] \), if the following condition holds for all \( m \in \mathcal{M} \):
\[
\Pr[\hat{M} = m | M = m] \geq 1 - \varepsilon_1.
\]

Equivalently, we require that
\[
\sup_{m \in \mathcal{M}} \left( 1 - \Pr[\hat{M} = m | M = m] \right) \leq \varepsilon_1.
\]

The protocol is \( \varepsilon_{II} \)-secret, with \( \varepsilon_{II} \in [0, 1] \), if for all channel states \( s \in \mathcal{S} \), there exists a fixed state \( \sigma_{ER}^s \) of Eve's systems, such that for all messages \( m \in \mathcal{M} \), the following inequality holds
\[
\frac{1}{2} \|\rho_{ER}^m - \sigma_{ER}^s\|_1 \leq \varepsilon_{II}.
\]

Equivalently, we require that
\[
\sup_{s \in \mathcal{S}} \sup_{m \in \mathcal{M}} \frac{1}{2} \|\rho_{ER}^m - \sigma_{ER}^s\|_1 \leq \varepsilon_{II}.
\]

Thus, for each \( s \in \mathcal{S} \), the protocol allows for sending a message securely, such that the eavesdropper cannot determine the message \( m \), no matter which channel \( \mathcal{N}_{X \to BE}^s \) is selected from \( \mathcal{S} \).

The number of private bits communicated by the scheme is equal to \( \log_2 |\mathcal{M}| \). Thus, a given protocol for private communication over the channel in (168) is described by the three parameters \( |\mathcal{M}|, \varepsilon_1, \) and \( \varepsilon_{II} \).

We remark that this setting reduces to the traditional one-shot, shared-randomness-assisted private communication setting considered in quantum information theoretic contexts in the case that \( |\mathcal{S}| = 1 \). See [Wil17a] for details of this special case.

### B. Distinguishability and information measures

Before stating Theorem 4 regarding the number of private messages that can be transmitted in the above setting, we briefly review the basic distinguishability measures and information quantities needed to understand the statement of Theorem 4.

Let \( \rho \) and \( \sigma \) be states acting on a separable Hilbert space \( \mathcal{H} \). The hypothesis testing relative entropy \( D_H^\varepsilon(\rho||\sigma) \) is defined for \( \varepsilon \in [0, 1] \) as [BD10, BD11, WR12]
\[
D_H^\varepsilon(\rho||\sigma) := -\log_{\Lambda \geq 0} \{\text{Tr}[\Lambda] : \text{Tr}[\Lambda \rho] \geq 1 - \varepsilon, \Lambda \leq I\}.
\]

Note that, without loss of generality, we can set the first constraint above to be an equality [KW17], so that
\[
D_H^\varepsilon(\rho||\sigma) := -\log_{\Lambda \geq 0} \{\text{Tr}[\Lambda] : \text{Tr}[\Lambda \rho] = 1 - \varepsilon, \Lambda \leq I\}.
\]

The max-relative entropy \( D_{max}(\rho||\sigma) \) is defined as
\[
D_{max}(\rho||\sigma) := \inf \{\lambda : \rho \leq \Lambda^\lambda \}.
\]

The following alternative characterization of \( D_{max}(\rho||\sigma) \) is well known [Dat09a]:
\[
D_{max}(\rho||\sigma) = \inf_{\lambda : \omega \geq 0} \{\lambda : \sigma = 2^{-\lambda} \rho + (1 - 2^{-\lambda}) \omega, \text{Tr}[\omega] = 1\},
\]

which allows for thinking of \( \sigma \) as a convex combination of \( \rho \) and some other state \( \omega \). The smooth max-relative entropy for \( \varepsilon \in [0, 1] \) is defined as [Dat09b]
\[
D_{max}^\varepsilon(\rho||\sigma) := \inf \{\lambda : \rho \leq \Lambda^\lambda, \rho \geq 0, \text{Tr}[\rho] = 1, P(\rho, \rho) \leq \varepsilon\}.
\]
where the sine distance \( P(\tilde{\rho}, \rho) \) is defined as [Ras02, Ras03, Ras06, GLN05]

\[
P(\tilde{\rho}, \rho) := \sqrt{1 - \frac{1}{2} F(\tilde{\rho}, \rho)}, \tag{189}
\]

\[
F(\tilde{\rho}, \rho) := \left\| \sqrt{\tilde{\rho}} \sqrt{\rho} \right\|_1^2, \tag{190}
\]

the latter quantity being the quantum fidelity [Uhl76].

Let \( \rho_{AE} \) be a state acting on a separable Hilbert space \( \mathcal{H}_A \otimes \mathcal{H}_E \). Then a mutual-information like quantity is defined for \( \varepsilon \in [0, 1] \) as

\[
D^\varepsilon_{\text{max}}(\rho_{AE} \| \rho_A \otimes \rho_E). \tag{191}
\]

We also define the alternate smooth max-mutual information as [AJW19b, Wil17a]

\[
\tilde{I}^\varepsilon_{\text{max}}(E; A)_\rho := \inf_{\tilde{\rho}_{AE} : P(\tilde{\rho}_{AE} \| \rho_{AE}) \leq \varepsilon} D^\varepsilon_{\text{max}}(\tilde{\rho}_{AE} \| \rho_A \otimes \rho_E). \tag{192}
\]

A simple relation between these two generalizations of mutual information is given in Appendix B. Note that we adopt the particular notation in (192) in order to maintain consistency with the notation of [BCR11].

The hypothesis testing mutual information of a bipartite state \( \rho_{AE} \) acting on a separable Hilbert space \( \mathcal{H}_A \otimes \mathcal{H}_B \) is defined for \( \varepsilon \in [0, 1] \) as [WR12]

\[
I_{\varepsilon}^H(A; B)_\rho := D^\varepsilon_{H}(\rho_{AB} \| \rho_A \otimes \rho_B). \tag{193}
\]

C. Private communication via position-based coding and convex splitting

The communication protocol that we develop here is the same as that considered in [Wil17a], but with the added observation that its security holds universally for any channel selected from the set \( \mathcal{S} \) and for channels whose output states act on a separable Hilbert space. The protocol from [Wil17a] built upon the ideas of position-based coding and convex splitting, which were in turn introduced in [AJW19b] and [ADJ17], respectively. Our main one-shot achievability theorem, for the communication setting described in Section III A, is as follows:

**Theorem 4** Fix \( \varepsilon_1, \varepsilon_2 \in (0, 1), \eta_1 \in (0, \varepsilon_1), \) and \( \eta_2 \in (0, \varepsilon_1) \). Then the following quantity is an achievable number of private message bits that can be transmitted over the compound wiretap channel in (168), with decoding error probability not larger than \( \varepsilon_1 \) and security parameter not larger than \( \varepsilon_2 \):

\[
\sup_{P_X} \left[ I_{\varepsilon_1}^{\eta_1}(X; B)_\rho - \sup_{s \in \mathcal{S}} \tilde{I}^{\varepsilon_2-\eta_1}_{\text{max}}(E; X)_{\rho^s} \right] \\
- \log_2(4 \varepsilon_1/\eta_1^2) - 2 \log_2(1/2 \eta_1), \tag{194}
\]

where the entropic quantities are evaluated with respect to the following state:

\[
\rho^s_{XBE} := \sum_{x \in \mathcal{X}} p_X(x) |x\rangle \langle x| \otimes \rho^s_{BE}. \tag{195}
\]

**Proof.** Consider the compound wiretap channel in (168). Let \( p_X \) be a probability distribution over the channel input alphabet \( \mathcal{X} \). Let \( \rho_{XX'X''} \) denote the following public shared randomness state:

\[
\rho_{XX'X''} := \sum_{x \in \mathcal{X}} p_X(x) |x\rangle \langle x| \otimes |x\rangle \otimes |x\rangle. \tag{196}
\]

We suppose that Alice, Bob, and Eve share the state

\[
\rho^{\otimes |M| |R|}_{XX'X''}, \tag{197}
\]

before communication begins and that the \( X \) systems are indexed as \( X_{m,r}, \ldots, X_{r,m} \), i.e., in lexicographic order by \( m \in \mathcal{M} \) and \( r \in \mathcal{R} \), where \( \mathcal{R} := \{1, \ldots, |\mathcal{R}|\} \). Alice possesses all of the \( X \) systems, Bob the \( X' \) systems, and Eve the \( X'' \) systems.

To send the message \( m \in \mathcal{M} \), Alice’s encoding consists of picking \( r \in \mathcal{R} \) uniformly at random from the set \( \mathcal{R} \), and then she sends the classical system \( X_{m,r} \) through the channel in (173). For fixed values of \( m, r, \) and \( s \), the global shared state at this point is given by

\[
\rho^s_{X_{m,r}, X'_{m,r}, X''_{m,r}} := \sum_{x \in \mathcal{X}} p_X(x) |x, x, x\rangle \langle x, x, x| \otimes \rho_{BE}^s. \tag{199}
\]

The resulting state of Bob, for fixed values \( m, r \), is as follows:

\[
\rho^s_{X_{m,r}} := \sum_{x \in \mathcal{X}} p_X(x) |x\rangle \langle x| \otimes \rho^s_{BE}. \tag{200}
\]

By employing the sequential and position-based decoding scheme from [OMW19] (which has been shown therein to hold for states acting on separable Hilbert spaces), it follows that Bob can decode both the message \( m \) and \( r \) with probability not smaller than \( 1 - \varepsilon_1 \) as long as

\[
\log_2(|\mathcal{M}| |\mathcal{R}|) = I^{\varepsilon_1-\eta_1}(X; B)_\rho - \log_2(4 \varepsilon_1/\eta_1^2), \tag{202}
\]

where \( \eta_1 \in (0, \varepsilon_1) \) and

\[
\rho_{XB} := \sum_{x \in \mathcal{X}} p_X(x) |x\rangle \langle x| \otimes \rho_{BE}. \tag{203}
\]
To Eve, who is unaware of the random choice of the local randomness variable \( r \in \mathcal{R} \), the state of her systems for a fixed value of the message \( m \) is as follows:

\[
\rho_{X^{(m)}|M|:E}^{r,s} := \frac{1}{|\mathcal{R}|} \sum_{r \in \mathcal{R}} \rho_{X^{(m)}_r|E}^{r,s} \otimes \rho_{X^{(m)}_{r+1}\ldots|E}^{r,s} \\
\otimes \rho_{X^{(m)}_{r+2}\ldots|E}^{r,s} (204)
\]

By the invariance of the trace distance with respect to tensor-product states, i.e., \( \| \sigma \otimes \tau - \omega \otimes \tau \|_1 = \| \sigma - \omega \|_1 \), we find that

\[
\frac{1}{2} \| \rho_{X^{(m)}|M|:E}^{r,s} - \rho_{X^{(m)}|M|:E} \|_1
= \frac{1}{2} \| \rho_{X^{(m)}_1\ldots|E}^{r,s} - \rho_{X^{(m)}_1\ldots} \otimes \rho_E \|_1 , (205)
\]

for any state \( \rho_E^{r} \). It follows from the smooth universal convex-split lemma (see Appendix C) that if

\[
\log_2 |\mathcal{R}| = \sup_{s \in S} \tilde{I}^{\epsilon_{II} - \eta_{II}}_{\text{max}}(E; X)_{\rho^r} + 2 \log_2(1/2\eta_{II}), (206)
\]

then the following bound holds for all \( m \in \mathcal{M} \) and for all \( s \in S \)

\[
\frac{1}{2} \| \rho_{X^{(m)}|M|:E}^{r,s} - \rho_{X^{(m)}|M|} \otimes \rho_E^{r,s} \|_1 \leq \epsilon_{II} , (207)
\]

where the state \( \rho_E^{r,s} \) satisfies \( P(\tilde{\rho}_E^{r,s}, \rho_E^{r,s}) \leq \epsilon_{II} - \eta_{II} \) and the alternate smooth max-mutual information \( \tilde{I}^{\epsilon_{II} - \eta_{II}}_{\text{max}}(E; X)_{\rho^r} \) is evaluated with respect to the state

\[
\rho_{X:E}^{s} := \sum_{x \in X} p_X(x)|x\rangle\langle x| \otimes \rho_{E}^{r,s}. (208)
\]

The analysis of this step is similar to that given in [Wil17a]. We provide details of the smooth universal convex-split lemma, as applicable to states acting on separable Hilbert spaces, in Appendix C. Thus, the number of private message bits that can be established with this scheme is equal to

\[
\log_2 |\mathcal{M}| = I^{\epsilon_1 - \eta_1}_{H}(X; B)_{\rho^r} - \sup_{s \in S} \tilde{I}^{\epsilon_{II} - \eta_{II}}_{\text{max}}(E; X)_{\rho^r} \\
- \log_2(4\epsilon_1/\eta_1^2) - 2 \log_2(1/2\eta_{II}). (209)
\]

Since the above number of private message bits is achievable for a fixed distribution \( p_X \), it is then possible to optimize over all distributions to conclude that it is possible to send the following number of private message bits:

\[
\log_2 |\mathcal{M}| = \\
\sup_{p_X} \left[ I^{\epsilon_1 - \eta_1}_{H}(X; B)_{\rho^r} - \sup_{s \in S} \tilde{I}^{\epsilon_{II} - \eta_{II}}_{\text{max}}(E; X)_{\rho^r} \right] \\
- \log_2(4\epsilon_1/\eta_1^2) - 2 \log_2(1/2\eta_{II}), (210)
\]

concluding the proof. □

Remark 5 If desired, this private communication scheme can be derandomized along the lines shown in [Wil17a], in order to end up with a scheme that does not require public shared randomness. After doing so, the protocol is no longer guaranteed to be secure against an arbitrary state of the eavesdropper in the uncertainty set \( \mathcal{S} \). The resulting protocol is only guaranteed to be secure against a fixed, known eavesdropper, similar to the standard information-theoretic model of private communication from [Dev05, CWY04].

IV. SECRET KEY DISTILLATION FROM A COMPOUND QUANTUM WIRETAP SOURCE WITH FIXED MARGINAL

A. One-shot setting

The setting of secret key distillation from a compound quantum wiretap source with fixed marginal can be considered the static version of the dynamic setting presented in Section III A, and so many aspects are similar. In this setting, we suppose that Alice has system \( X \), Bob system \( B \), and Eve system \( E \) of the following classical–quantum–quantum compound wiretap source state with fixed marginal:

\[
\rho_{XBE}^x := \sum_x p_X(x)|x\rangle\langle x| \otimes \rho_{BE}^{r,s}, (211)
\]

where \( s \in \mathcal{S} \). In this model, the marginal state of Alice and Bob is fixed, such that they know their reduced state \( \rho_{XB}^x \). That is,

\[
\rho_{BE}^{r,s} = \rho_{BE} \quad \text{for all} \quad s \in \mathcal{S}, (212)
\]

but they do not know the full state. We suppose that forward public classical communication from Alice to Bob is allowed for free. The goal is to use this compound wiretap source state in (211), along with the free public classical communication, in order to distill a key that is secure for all \( \rho_{XBE}^x \) and \( s \in \mathcal{S} \).

A secret key distillation scheme consists of a classical encoding channel \( \tilde{\mathcal{X}}_{K \rightarrow KL} \) and a decoding channel \( \mathcal{D}_{LB \rightarrow K} \). In the above, \( K \) is the classical key register of Alice and \( L \) is a classical register communicated to Bob. Two parameters \( \epsilon_1 \) and \( \epsilon_{II} \) determine the error probability when decoding and the security of the protocol, respectively. Alice uses the distillation scheme and the state in (211) to produce a uniformly random key \( \hat{K} \) to \( K \) (the probability \( \Pr[\hat{K} = K] = 1/|\mathcal{K}| \)), and the conditional probability of Bob decoding \( k' \in K \) from his systems is given by

\[
\Pr[\hat{K} = k'|K = k] := \langle k'| \mathcal{D}_{LB \rightarrow K}(\rho_{KLB}^k)|k'\rangle_{\hat{K}}, (214)
\]
where

\[ \rho_{KLB}^k := \text{Tr}_E \rho_{LB}^{k,\Phi}, \]
\[ \rho_{KLB}^{k,s} := \frac{(k|k_EX\rightarrow KL(\rho_{XBE})|k)_K}{\text{Pr}[K = k]}, \]
\[ = (k|k_EX\rightarrow KL(\rho_{XBE})|k)_K : |K|. \]

Alternatively, we can consider Bob’s positive operator-valued measure \( \{\Lambda_{LB}^k\}_{k \in K} \) to consist of the following elements

\[ \Lambda_{LB}^k := (\mathcal{D}_{LB\rightarrow K})^\dagger(|k|\Phi)_K, \]

where \( (\mathcal{D}_{LB\rightarrow K})^\dagger \) is the Hilbert–Schmidt adjoint of the decoding channel \( \mathcal{D}_{LB\rightarrow K} \), so that we can write the probability \( \text{Pr}[\hat{K} = k'|K = k] \) in terms of the Born rule as

\[ \text{Pr}[\hat{K} = k'|K = k] = \text{Tr}[\Lambda_{LB}^k \rho_{KLB}^k]. \]

The protocol is \( \epsilon_1 \)-reliable, with \( \epsilon_1 \in [0, 1] \), if the following condition holds for all \( k \in K \):

\[ \text{Pr}[\hat{K} = k|K = k] \geq 1 - \epsilon_1. \]

Equivalently, we require that

\[ \sup_{k \in K} \left( 1 - \text{Pr}[\hat{K} = k|K = k] \right) \leq \epsilon_1. \]

The protocol is \( \epsilon_{II} \)-secret, with \( \epsilon_{II} \in [0, 1] \), if for all source values \( s \in S \), there exists fixed state \( \sigma_{E|RE}^s \) of Eve’s systems, such that for all key values \( k \in K \), the following inequality holds

\[ \frac{1}{2} \left\| \rho_{LE}^{k,s} - \sigma_{LE}^s \right\|_1 \leq \epsilon_{II}. \]

Equivalently, we require that

\[ \sup_{s \in S} \inf_{k \in K} \sup_{\kappa \in K} \frac{1}{2} \left\| \rho_{LB}^{k,s} - \rho_{LE}^{k,s} - \sigma_{LE}^s \right\|_1 \leq \epsilon_{II}. \]

Thus, for each \( s \in S \), the protocol allows for distilling a secure key no matter which state \( \rho_{E|RE}^{s} \) is selected from \( S \).

The number of key bits established by the scheme is equal to \( \log_2 |K| \). Thus, a given protocol for secret key distillation using the source in (211) is described by the three parameters \( |K|, \epsilon_1, \) and \( \epsilon_{II} \).

We remark here that the definition given above implies the usual trace-distance based criterion [KRBM07, TLGR12] for security that is commonly employed in quantum key distribution. Let \( K \) and \( \hat{K} \) denote the respective classical key registers of Alice and Bob (we identify both the random variable and the system label with the same symbol). Then the final state of the protocol, for fixed \( s \in S \), can be written as follows:

\[ \rho_{K\hat{K}LE}^{s} := \sum_k \frac{1}{|K|} (k|k|K \otimes \sum_{k'} p(k'|k)|k'|\hat{K} \otimes \rho_{LE}^{k,s}), \]

where \( p(k'|k) := \text{Tr}[\Lambda_{LB}^{k'} \rho_{KLB}^{k} \otimes \Phi], \) while the ideal state, for the same \( s \), is as follows:

\[ \tilde{\Phi}_{KK} \otimes \sigma_{LE}^s, \]

for some fixed state \( \sigma_{LE}^s \) and where \( \tilde{\Phi}_{KK} := \sum_k |k|k|K \otimes |k|k|\hat{K}. \) The conditions in (220) and (223) and the triangle inequality for trace distance imply that

\[ \frac{1}{2} \left\| \rho_{K\hat{K}LE}^{s} - \text{Tr} \rho_{K\hat{K}LE}^{s} - \tilde{\Phi}_{KK} \otimes \sigma_{LE}^s \right\|_1 \leq \epsilon_1 + \epsilon_{II}. \]

Equivalently, we require

\[ \sup_{s \in S} \inf_{k \in K} \frac{1}{2} \left\| \rho_{K\hat{K}LE}^{s} - \tilde{\Phi}_{KK} \otimes \sigma_{LE}^s \right\|_1 \leq \epsilon, \]

which is the standard trace-distance based criterion considered in the context of secret key distillation [TLGR12]. As pointed out in [TLGR12, PR14], however, this criterion is not composable. The criterion that is known to be composable is

\[ \sup_{s \in S} \inf_{k \in K} \frac{1}{2} \left\| \rho_{K\hat{K}LE}^{s} - \tilde{\Phi}_{KK} \otimes \rho_{LE}^{s} \right\|_1 \leq \epsilon, \]

where \( \rho_{LE}^{s} := \text{Tr}_E [\Lambda_{LB}^{s} \rho_{KLB}^{s}] \). As shown in [PR14, Appendix B], if the criterion in (227) is satisfied, then (228) is satisfied with \( \epsilon = 2(\epsilon_1 + \epsilon_{II}) \).

We end this section by remarking that this setting reduces to the traditional one-shot, secret key distillation setting from a known source, considered in quantum information-theoretic contexts [RR12], in the case that \( |S| = 1 \).

**B. Secret key distillation via position-based coding and convex splitting**

Our main one-shot achievability theorem, corresponding to the key distillation setting discussed in the previous section, is as follows:

**Theorem 6** Fix \( \epsilon_1, \epsilon_{II} \in (0, 1), \eta_1 \in (0, \epsilon_1), \) and \( \eta_{II} \in (0, \epsilon_{II}) \). Then the following quantity is an achievable number of secret key bits that can be distilled from the compound wiretap source in (211), with decoding error probability not larger than \( \epsilon_1 \) and security parameter not larger than \( \epsilon_{II} \):

\[ I_{H}^{\epsilon_1-\eta_1}(X;B)\rho - \sup_{s \in S} \tilde{I}_{\text{max}}^{\epsilon_1-\eta_1}(E;X)_{\rho}, \]

\[ - \log_2 (4\epsilon_1/\eta_1^2) - 2 \log_2 (1/2\eta_1), \]

where the entropic quantities are evaluated with respect to the state in (211).

**Proof.** The secret key distillation scheme consists of the following steps. Alice, Bob, and Eve begin with the
classical–quantum–quantum state in (211). Alice picks a value \( k \in \mathcal{K} \) uniformly at random, and she picks a value \( r \in \mathcal{R} \) uniformly at random, where \( \mathcal{R} := \{1, \ldots, |\mathcal{R}|\} \). She then labels her X system of the state in (211) by the pair \((k, r)\), as \(X_{k, r}\). She prepares \(|\mathcal{K}| |\mathcal{R}| - 1\) independent instances of the classical state
\[
\rho_X = \sum_{x \in \mathcal{X}} \rho_X(x|x)\]  
and labels the systems as \(X_{1,1}, \ldots, X_{k, r-1}, X_{k, r+1}, \ldots, X_{|\mathcal{K}| |\mathcal{R}|}\). Alice sends the classical registers \(X_{1,1}, \ldots, X_{|\mathcal{K}| |\mathcal{R}|}\) in lexicographic order over a public classical communication channel, so that Bob and Eve receive copies of them. For fixed values of \(k, r, s\), the global shared state at this point is given by
\[
\begin{align*}
p^{k, r, s}_{X|\mathcal{K}| |\mathcal{R}| |\mathcal{X}} := & \rho_{X_{1,1}, \ldots, X_{k, s-1}, X_{k, s}, X_{k, s+1}, \ldots, X_{|\mathcal{K}| |\mathcal{R}|}} \\
&\otimes \rho_{X_{k, r+1}, \ldots, X_{k, r-1}, X_{k, r}, B} \\
&\otimes \rho_{X_{k, r+1}, \ldots, X_{k, r-1}, X_{k, r}, E} \\
&\otimes \rho_{X_{k, r+1}, \ldots, X_{k, r-1}, X_{k, r}, E} \\
&\otimes \rho_{X_{k, r+1}, \ldots, X_{k, r-1}, X_{k, r}, E}.
\end{align*}
\]  
Thus, the reduced state of Bob, for fixed \(k, r\), is as follows:
\[
\begin{align*}
p^{k, r}_{X|\mathcal{K}| |\mathcal{R}| |\mathcal{X}} & := \rho_{X_{1,1}, \ldots, X_{k, s-1}, X_{k, s}, X_{k, s+1}, \ldots, X_{|\mathcal{K}| |\mathcal{R}|}} \\
&\otimes \rho_{X_{k, r+1}, \ldots, X_{k, r-1}, X_{k, r}, B} \\
&\otimes \rho_{X_{k, r+1}, \ldots, X_{k, r-1}, X_{k, r}, E} \\
&\otimes \rho_{X_{k, r+1}, \ldots, X_{k, r-1}, X_{k, r}, E} \\
&\otimes \rho_{X_{k, r+1}, \ldots, X_{k, r-1}, X_{k, r}, E}.
\end{align*}
\]  
The reduced state of Eve, for a fixed value of \(k\) and \(s\), is as follows:
\[
\begin{align*}
p^{k, s}_{X|\mathcal{K}| |\mathcal{R}| |\mathcal{X}} & := \frac{1}{|\mathcal{R}|} \sum_{r \in \mathcal{R}} \rho_{X_{1,1}, \ldots, X_{k, s-1}, X_{k, s}, X_{k, s+1}, \ldots, X_{|\mathcal{K}| |\mathcal{R}|}} \\
&\otimes \rho_{X_{k, r+1}, \ldots, X_{k, r-1}, X_{k, r}, E} \\
&\otimes \rho_{X_{k, r+1}, \ldots, X_{k, r-1}, X_{k, r}, E} \\
&\otimes \rho_{X_{k, r+1}, \ldots, X_{k, r-1}, X_{k, r}, E} \\
&\otimes \rho_{X_{k, r+1}, \ldots, X_{k, r-1}, X_{k, r}, E}.
\end{align*}
\]  
These reduced states are exactly the same as they are in (200) and (204), and so the same analysis applies. Bob decodes both the key value \(k\) and the local randomness value \(r\) with success probability not smaller than \(1 - \varepsilon_1\), as long as
\[
\log_2(|\mathcal{K}| |\mathcal{R}|) = I_{\mathcal{K}}^{\varepsilon_1 - \eta_1}(X; B) - \log_2(4\varepsilon_1/\eta_1^2),
\]  
while the following security condition holds for all \(k \in \mathcal{K}\) and \(s \in \mathcal{S}\):
\[
\frac{1}{2} \left\| p^{k,s}_{X|\mathcal{K}| |\mathcal{R}| |\mathcal{X}} - \rho_{X|\mathcal{K}| |\mathcal{R}|} \otimes \tilde{\rho}_E \right\|_1 \leq \varepsilon_1, \]  
for some state \(\tilde{\rho}_E\), as long as
\[
\log_2 |\mathcal{R}| = \sup_{s \in \mathcal{S}} \tilde{I}_{\mathcal{K}}^{\varepsilon_1 - \eta_1}(E; X)_{\rho^s} + 2 \log_2(1/2\eta_1). \]  
Thus, the number of key bits that can be established with this scheme is equal to
\[
\log_2 |\mathcal{K}| = I_{\mathcal{K}}^{\varepsilon_1 - \eta_1}(X; B)_{\rho} - \sup_{s \in \mathcal{S}} \bar{I}_{\mathcal{K}}^{\varepsilon_1 - \eta_1}(E; X)_{\rho^s} - \log_2(4\varepsilon_1/\eta_1^2) - 2 \log_2(1/2\eta_1), \]  
as claimed.

\section{V. Second-Order Asymptotics of Private Communication and Secret Key Distillation}

In this section, we show how to apply the one-shot results from Sections III and IV to the case of independent and identically distributed (i.i.d.) resources. First, let us suppose that Alice, Bob, and Eve are connected by means of a cq compound wiretap channel of the form in (168):
\[
N_{X \rightarrow BE}^n : x \rightarrow \rho_{BE}^{x,s},
\]  
with all the same assumptions discussed previously in Section III A. However, now we allow them to use the channel multiple times, and we suppose that the particular value of \(s\) is fixed but unknown for all channel uses. Thus, the resource they are employing for private communication is the tensor-power channel \((N_{X \rightarrow BE}^n)^{\otimes n}\), where \(n\) is a large positive integer. This setting is directly related to a collective attack in quantum key distribution, as discussed in Section II.

By applying the result of Theorem 4 to this setting, invoking Lemma 7 and the second-order asymptotic expansions discussed in (F5) and Corollary 11, with \(\eta_1 = \eta_{11} = 1/\sqrt{n}\), we find that it is possible to send private message bits at the following rate, for sufficiently large \(n\), with decoding error probability not larger than \(\varepsilon_1\) and security parameter not larger than \(\varepsilon_{11} n\):
\[
\frac{\log_2 |\mathcal{M}|}{n} = \sup_{x} I(X; B)_{\rho^x} + \sqrt{\frac{1}{n} V(X; B)_{\rho} \Phi^{-1}(\varepsilon_1)} \\
- \sup_{s \in \mathcal{S}} \left[ I(X; E)_{\rho^s} - \sqrt{\frac{1}{n} V(X; E)_{\rho^s} \Phi^{-1}(\varepsilon_{11}^2)} \right] + O\left(\frac{\log n}{n}\right). \]  
In the above, the information quantities are evaluated with respect to the following classical–quantum state:
\[
\rho_{BE} := \sum_x \rho_X(x|x)x \otimes \rho_{BE}^{x,s},
\]  
and
\[
I(X; B)_{\rho} := \sum_x p_X(x)D(\rho_B^x\|\rho_B), \]  
\[
I(X; E)_{\rho^s} := \sum_x p_X(x)D(\rho_E^{x,s}\|\rho_E^s), \]  
\[
\rho_B := \sum_x p_X(x)\rho_B^x, \]  
\[
\rho_E := \sum_x p_X(x)\rho_E^{x,s}. \]

The Holevo information variances \(V(X; B)_{\rho}\) and \(V(X; E)_{\rho^s}\) are given by
\[ V(X; B)_{\rho} := \sum_{x \in X} p_X(x) \left[ V(\rho_B^{x_{\rho}} \| \rho_B) + [D(\rho_B^{x_{\rho}} \| \rho_B)]^2 \right] - [I(X; B)_{\rho}]^2, \]
\[ (245) \]

\[ V(X; E)_{\rho'} := \sum_{x \in X} p_X(x) \left[ V(\rho_E^{x_{\rho'}} \| \rho_E) + [D(\rho_E^{x_{\rho'}} \| \rho_E)]^2 \right] - [I(X; E)_{\rho'}]^2, \]
\[ (246) \]

with these formulas considered in more detail in Appendix G. The term \( O(\log n) \) hides constants involving \( \varepsilon_1, \varepsilon_\Pi, T(X; B)_{\rho}, \) and \( T(X; E)_{\rho'} \), with the latter two quantities defined in Appendix G. By noting that all of the quantities \( I(X; B)_{\rho}, I(X; E)_{\rho'}, V(X; B)_{\rho}, V(X; E)_{\rho'}, T(X; B)_{\rho}, \) and \( T(X; E)_{\rho'} \) involve an expectation with respect to the distribution \( p_X \), it follows from an approximation argument that the same formula in (239) is an achievable rate for private communication when \( p_X \) is a probability distribution over a continuous alphabet. In this case, all of the expectations for the various quantities are evaluated by integration.

In the case that the states involved in the above formulas act on separable Hilbert spaces, then we should define the various quantities in more detail because the formulas in (38) and (39) need to be interpreted in a particular way (that is, the trace cannot be taken with respect to an arbitrary orthonormal basis). Suppose that \( \rho \) and \( \sigma \) have the following spectral decompositions:

\[ \rho = \sum_x \lambda_x |\psi_x \rangle \langle \psi_x|, \quad \sigma = \sum_y \mu_y |\phi_y \rangle \langle \phi_y|. \]
\[ (247) \]

Then the quantum relative entropy [Fal70, Lin73] and the relative entropy variance [TH13, Li14, KW17] are defined as

\[ D(\rho \| \sigma) := \sum_{x, y} |\langle \phi_y | \psi_x \rangle|^2 \lambda_x \log_2 \left( \frac{\lambda_x}{\mu_y} \right), \]
\[ (248) \]

\[ V(\rho \| \sigma) := \sum_{x, y} |\langle \phi_y | \psi_x \rangle|^2 \lambda_x \left[ \log_2 \left( \frac{\lambda_x}{\mu_y} \right) - D(\rho \| \sigma) \right]^2. \]
\[ (249) \]

We can also consider the application to secret key distillation. Suppose now that Alice, Bob, and Eve share \( n \) copies of the following cqq state:

\[ \rho_{XBE} := \sum_x p_X(x) |x \rangle \langle x| \otimes \rho_{BE}^{x_{\rho}}, \]
\[ (250) \]

with all of the same assumptions discussed previously in Section IV B. Then by the same reasoning as given above, but this time applying Theorem 6, the following formula represents an achievable rate for secret key distillation, for sufficiently large \( n \) and with decoding error probability not larger than \( \varepsilon_1 \) and security parameter not larger than \( \varepsilon_\Pi \):

\[ \log_2 \left( \frac{K}{n} \right) = I(X; B)_{\rho} + \sqrt{\frac{1}{n} [V(X; B)_{\rho}]^2} \]
\[ - \sup_{s \in S} \left[ I(X; E)_{\rho'} - \sqrt{\frac{1}{n} [V(X; E)_{\rho'}]^2} \right] + O \left( \log n \right), \]
\[ (251) \]

where all information quantities are evaluated with respect to the state in (250).

VI. DISCUSSION OF COLLECTIVE ATTACKS IN QKD AND THE COMPOUND WIRETAP CHANNEL AND SOURCE

As mentioned in the introduction, from what we can gather by combing through the literature, it seems that there is a disconnect between the community of researchers working on security proofs against collective attacks in quantum key distribution and those working on key distillation from a compound wiretap source. Thus, one contribution of this paper is to connect these two research directions, with Theorem 6 and its applications in Sections II and V providing a direct link between them.

The main purpose of this section is to trace some of the historical developments and early roots of these disparate communities. This might help with unifying them going forward. To begin with, let us note that there are several reviews of quantum key distribution in which collective attacks are discussed [SBPC+09, Lit14, DLQY16, XMZ+19]. Furthermore, there is a recent review of the compound wiretap channel that traces its development in classical information theory [SBP15].

The compound channel for classical communication was introduced in [BBT59, Wol59]. The basic idea here is that the actual communication channel is chosen from an uncertainty set \( \{ p_{XY|1} \} \), which is the same over a large block-length (used in an i.i.d. way), and the goal is to be able to communicate regardless of which channel is selected. The main result of [BBT59, Wol59] is that Shannon’s formula for capacity becomes modified to

\[ \max_{p_X} \min_s I(X; Y)_p, \]
\[ (252) \]

where \( p^{s}_{XY} = p_X p_{Y|X}^{s} \).

The classical wiretap channel \( p_{YZ|X} \) and its private capacity were introduced in [Wyn75] and studied further by [CK78, Csi96, MW00]. In this model, the sender inputs the random variable \( X \), the legitimate receiver obtains \( Y \), and the wiretapper (eavesdropper) \( Z \). The conditional probability distribution \( p_{YZ|X} \) is known to all parties involved. The culmination of these papers was to identify the formula

\[ \max_{U \rightarrow X \rightarrow Y Z} \left[ I(U; Y) - I(U; Z) \right] \]
\[ (253) \]

as the private capacity of an arbitrary classical wiretap channel. The optimization is over Markov chains.
\( U \rightarrow X \rightarrow Y Z \), where \( U \) is known as an auxiliary random variable. Interestingly, this formula provides the insight that noise at the encoder (the channel from \( X \) to \( U \)) can increase private capacity, with the reasoning being that, even though it decreases both informations \( I(U; Y) \) and \( I(U; Z) \), it can happen that it decreases the wiretapper’s information \( I(U; Z) \) by more, so that there can be a noise benefit. The main reason why the classical wiretap channel model has not been embraced by the classical cryptography community is that the model assumes that the channel to the eavesdropper is known, and this is too much to assume in practice. Interestingly, it would be some years before the compound wiretap channel and source were defined.

The source model for secret key agreement was introduced by [AC93]. In this model, two legitimate parties have access to respective random variables \( X \) and \( Y \) and an eavesdropper has access to a random variable \( Z \) described by the joint probability distribution \( p_{XYZ} \), and the legitimate parties are allowed public classical communication. All parties know the distribution \( p_{XYZ} \). If public classical communication is allowed only in one round from \( X \) to \( Y \), then the secret key agreement capacity is given by the formula [AC93]

\[
\max_{p_{UV|X}} [I(V; Y|U) - I(V; Z|U)].
\]

In independent work, it was shown that public communication can enhance the secret key agreement capacity of a wiretap channel [Man93], and an upper bound on the secret key agreement capacity was established in the case that arbitrary public classical communication is allowed.

The notion of a collective attack in quantum key distribution was proposed by [BBB], and further studied in [BBB]. Quantum de Finetti theorems and their variants were proved [Ren05, CKR09], which demonstrate that general coherent (arbitrary) attacks are no better than collective attacks in the limit of large blocklength. Quantum de Finetti theorems thus establish the significance of focusing on collective attacks in the context of quantum key distribution.

The quantum wiretap channel was proposed and studied in [Dev05, CWY04]. In this model, the wiretap channel is given by \( x \rightarrow \rho^BE \), with the sender having access to the input, the legitimate receiver to the quantum system \( B \), and the eavesdropper to the quantum system \( E \). It is assumed that the full channel is known to both the sender and legitimate receiver. An important result from [Dev05, CWY04] is that

\[
\max_{U \rightarrow X} [I(U; B) - I(U; E)]
\]

is an achievable rate at which they can communicate privately, paralleling the formula in (253) for the classical case. It is not known whether this achievable rate is optimal in general. That is, it is an open problem to determine the private capacity of the classical–quantum wiretap channel in the general case.

The quantum wiretap source was proposed and studied in [DW05]. The model is that Alice, Bob, and Eve share a state of the form \( \sum_x p(x) |x⟩⟨x| \otimes \rho^BE \), and the goal is to use many copies of this state along with public classical communication in order to distill a secret key. The authors of [DW05] found that the rate

\[
I(X; B) - I(X; E)
\]

is achievable for key distillation using many copies of the aforementioned state. It is important to stress that, in this model, it is assumed that Alice and Bob have full knowledge of the state, including the state of the eavesdropper. For this reason, it is not justified to apply the formula in (256) generally when analyzing the security of quantum key distribution against collective attacks. In the special case that the quantum key distribution protocol involves preparations and measurements that are tomographically complete, the legitimate parties determine the state of the eavesdropper up to an information-theoretically irrelevant isometry, and it is then justified to apply the formula in (256) for security against collective attacks.

The classical compound wiretap channel was proposed and studied in [LKPS09] and studied further in [BBS13] (see also [SBP15] for a review). The model is that the actual wiretap channel is chosen from an uncertainty set \( \{ p_{YZ|X} \}_s \), it is the same over a large blocklength (used in an i.i.d. way), and the goal is to be able to communicate privately regardless of which channel is selected. One critical result of [LKPS09] is that the following formula is an achievable rate for private communication in this setting, when the uncertainty set is finite:

\[
\max_{U \rightarrow X \rightarrow Y Z} \left[ \min_s I(U; Y_s) - \max_s I(U; Z_s) \right].
\]

The classical compound wiretap channel model is more acceptable from a cryptographic perspective than is the standard wiretap channel model, because it allows for uncertainty in the channel to the wiretapper. However, it is still difficult to argue that anything about the channel to the wiretapper would be known in a fully classical context.

The classical compound wiretap source was considered in [BW13] and further studied in [TBS17]. The special case of a classical compound source with one fixed marginal was considered previously in [Blo10]. The model from [BW13, TBS17] is that two legitimate parties and an eavesdropper share a source chosen from an uncertainty set \( \{ p_{XYZ} \}_s \), and they are allowed public classical communication to assist in the task of distilling a secret key. In [TBS17], a formula for the achievable distillable secret key was given, and we refer to [TBS17] for the details. In the special case that the marginals \( X \) and \( Y \) are fixed, the results of [Blo10, TBS17] imply that the rate

\[
I(X; Y) - \max_s I(X; Z)
\]
is achievable for key distillation.

The compound quantum wiretap source was proposed and studied in [BJ16]. The model studied there is that the legitimate parties and the eavesdropper share a state \( \rho_{XBE} = \sum_x p(x) x^{\otimes x} \otimes \rho_{BE}^s \) selected from an uncertainty set \( \{ \rho_{BE}^s \}_s \), and the goal is to use one round of forward public classical communication from X to B in order to distill a secret key. In [BJ16], a formula for the achievable distillable secret key was given, and we refer to [BJ16] for the details. In the special case that the marginals X and B are fixed, the results of [BJ16] imply that the rate

\[
I(X; B) - \max_s I(X; E)
\]

is achievable. An even further special case is when the B system is classical. Thus, the results of [BJ16] can be used to analyze the security of quantum key distribution against collective attacks. This model is acceptable from a cryptographic setting because one can determine the uncertainty set for the state of the eavesdropper during the parameter estimation round of a quantum key distribution protocol. This is possible under the assumption that the eavesdropper is constrained by the laws of quantum mechanics and due to the structure of quantum mechanics. One of the contributions of our paper is to extend these results (with fixed marginal on X and B) to a second-order coding rate and have the formula apply to infinite-dimensional systems of interest in continuous-variable quantum key distribution.

The compound quantum wiretap channel was presented in [DH10, BCCD14]. In [DH10], the model is that the wiretap channel is selected from an uncertainty set \( x \rightarrow \rho_{BE}^s \) indexed by s, the channel is the same over the whole blocklength (used in an i.i.d. way), and the goal is to communicate privately to the legitimate receiver B regardless of which channel is selected from the set. It is unclear whether the claims of [DH10] hold as generally as stated therein, but in the case that public shared randomness is available to the legitimate parties, then the claims of [DH10] appear to hold. The main issue with the claims of [DH10] is that the code is derandomized, and when this is done, it is no longer the case that the code is secure against all of the possible states of the adversaries, as claimed therein. One would need to apply a union bound argument, as is done in [BCCD14, Section IV]. However, this issue does not arise if the code is not derandomized (in the case that the legitimate parties have public shared randomness). The coding scheme of [DH10] is universal in the sense that all that is required for communication is a lower bound on the Holevo information with the legitimate receiver and an upper bound on the Holevo information with the wiretapper. The paper [BCCD14] considered the same model, but with the uncertainty set being known and finite. They found that the following rate is achievable for private communication in this setting:

\[
\max_{U \rightarrow X \rightarrow B, E_s} \left[ \min_s I(U; B_s) - \max_s I(U; E_s) \right],
\]

representing a quantum generalization of the main result of [LKPS09].

Going forward from here, it would be interesting to develop the compound wiretap channel and source in more detail, in order to extend the scope of the results and given the applicability to key distillation in quantum key distribution. This is one contribution of the present paper, since we have established second-order coding rates for compound wiretap channels and sources for infinite-dimensional quantum systems when there is a fixed marginal. Furthermore, the quantum key distribution application is well motivated from a cryptographic perspective, given that it is possible to constrain the possible states (uncertainty set) of an eavesdropper who operates according to the laws of quantum mechanics. This is a critical difference with the classical compound wiretap channel, in which it is not possible to do so.

A. Remarks on the Devetak–Winter formula and security against collective attacks

We now comment briefly on the use of the Devetak–Winter argument in the context of collective attacks in quantum key distribution. The formula in (259) has been consistently employed by the quantum key distribution community as an achievable rate for distillable key against collective attacks. This formula is indeed correct. However, as discussed above, the argument of [DW05] did not justify this formula. Instead, it argued for the achievability of (259) when there is a known collective attack, which is applicable in the case that the preparation and measurement procedure in a QKD protocol is tomographically complete. Specifically, one can analyze the proof of [DW05, Theorem 2.1] to see that the key distillation scheme constructed ends up depending on the state shared by all three parties and security is only guaranteed in this case. From what we can tell, the formula in (259) was first proven by [RGK05] for the qubit case and then in [Ren05, Corollary 6.5.2] for general finite-dimensional states. The latter case has also been considered in [BJ16]. For infinite-dimensional states, the present paper has established a proof that the formula in (259) is achievable.

VII. OTHER CONTRIBUTIONS

In this section, we briefly list some other consequences of our work. First, the task of entanglement-assisted private communication over a broadcast channel was considered recently in [QSW18]. The technique behind the proof of Theorem 4 applies to this setting, allowing for protection against a quantum wiretap channel with fixed marginal to the decoding set. The result also applies to the infinite-dimensional case (separable Hilbert spaces).

We can also combine the techniques from Theorem 4 with those in [AJW19a, Theorem 1] and [Sen18, Corol-
VIII. CONCLUSION

In this paper, we have provided a second-order analysis of quantum key distribution as a bridge between the asymptotic and non-asymptotic regimes. The technical contributions that allowed for this advance are a coding theorem for one-shot key distillation from a compound quantum wiretap source with fixed marginal, as well as the establishment of the second-order asymptotics for the smooth max-relative entropy. Another contribution is a coding theorem for private communication over a compound quantum wiretap channel with fixed marginal. We also showed how to optimize the second-order coding rate for several exemplary QKD protocols, including six-state, BB84, and continuous-variable QKD. In Section VII, we briefly mentioned several other immediate applications of our technical results.

Going forward from here, an important open problem is to provide a full second-order analysis of both the parameter estimation and key distillation steps of a quantum key distribution protocol. At the moment, we have exclusively analyzed second-order coding rates for the key distillation step, under the assumption that the parameter estimation step provides reliable estimates. It seems plausible to incorporate the latest developments from [Hay19], in combination with the methods of this paper, in order to have a complete second-order analysis of both parameter estimation and key distillation.

Another practical concern is to reduce the amount of public shared randomness that the protocol from Theorem 4 employs. Likewise, it would be ideal to reduce the amount of public classical communication used by the protocol from Theorem 6. Even though these resources are typically considered essentially free in a private communication setting, it would still be ideal to minimize their consumption. We note here that this large usage of a free resource is typical of the methods of position-based coding [AJW19b] and convex splitting [ADJ17], which seems to be the cost for obtaining such simple formulas in the one-shot case. Recent work in other domains has shown how to reduce the amount of free resource that these kinds of protocols consume [Anshu18].

We think it would also be interesting to consider secret key distillation in the setting of private communication per unit cost from [DPW19]. It seems likely that the key distillation protocol given in Theorem 6 could be helpful for this task.

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[Nota] In some QKD protocols, the entire joint distribution of Alice’s and Bob’s classical data $p_{XY}(x,y)$ need not be estimated in order to distill a secure key. A well known example is CV-QKD, where only two scalar parameters need to be estimated in order to derive a key-rate lower bound under a collective-attack assumption, even in a finite key-length regime [Lev15]. It is possible that, for such protocols, the second-order correction to the key distillation rate that we present in this paper could be extended to a formulation that does not require the estimation of $p_{XY}(x,y)$.

[Notb] When estimating $p_{Y|X}$, we can bin the outcomes of the joint distribution $p_{XY}$ to get a discrete distribution $p_{X,Y|n}$ instead. Then we can estimate this finite distribution $p_{X,Y|n}$ instead, which is reasonable since there are a finite number of parameters, and plug the values into the classical mutual information $I(X_{m};Y_{n})$ and classical mutual information variance $V(X_{m};Y_{n})$ for a second-order coding rate for information reconciliation. Then the limits $I(X_{m};Y_{n}) \rightarrow I(X;Y)$ and $V(X_{m};Y_{n}) \rightarrow V(X;Y)$ hold as the bin size gets smaller.

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**Appendix A: Mutual and Holevo informations and variances for six-state and BB84 protocols**

When Alice and Bob discard their basis information in the six-state or BB84 protocols, then their classical data can be described via the following quantum channel:

$$N_{A \rightarrow B}(\rho_A) = p_1 \rho_A + p_2 Z \rho_A Z + p_3 X \rho_A X + p_4 Y \rho_Y,$$  

(A1)

where $p_1, p_2, p_3, p_4 \geq 0$, $p_1 + p_2 + p_3 + p_4 = 1$, and there are further constraints on $p_1, p_2, p_3, p_4$.

For the six-state protocol,

$$p_1 = 1 - \frac{3Q}{2},$$  

(A2)

$$p_2 = p_3 = p_4 = \frac{Q}{2},$$  

(A3)

$$Q = \frac{1}{3} (Q_x + Q_y + Q_z).$$  

(A4)

For these values of $p_1, p_2, p_3, p_4$, we obtain

$$p_{XY}(0, 0) := \frac{1}{2} \text{Tr}[|0\rangle\langle 0| B N_{A \rightarrow B}(|0\rangle\langle 0| A)]$$  

(A5)

$$= \frac{1}{2} (1 - Q),$$  

(A6)

$$p_{XY}(0, 1) := \frac{1}{2} \text{Tr}[|1\rangle\langle 1| B N_{A \rightarrow B}(|0\rangle\langle 0| A)]$$  

(A7)

$$= \frac{1}{2} Q,$$  

(A8)

$$p_{XY}(1, 0) := \frac{1}{2} \text{Tr}[|0\rangle\langle 0| B N_{A \rightarrow B}(|1\rangle\langle 1| A)]$$  

(A9)

$$= \frac{1}{2} Q,$$  

(A10)

$$p_{XY}(1, 1) := \frac{1}{2} \text{Tr}[|1\rangle\langle 1| B N_{A \rightarrow B}(|1\rangle\langle 1| A)]$$  

(A11)

$$= \frac{1}{2} (1 - Q),$$  

(A12)

which is consistent with the probability distribution $P_{X \rightarrow Y}$ in (109)–(112).

For the BB84 protocol,

$$p_1 = 1 - 2Q + s,$$  

(A13)

$$p_2 = Q - s,$$  

(A14)

$$p_3 = Q - s,$$  

(A15)

$$p_4 = s,$$  

(A16)

$$Q = \frac{1}{2} (Q_x + Q_z),$$  

(A17)

$$s = Q - \frac{Q_y}{2},$$  

(A18)

where $s \in [0, Q]$ is a parameter to be optimized. Indeed, for these values of $p_1, p_2, p_3, p_4$,

$$p_{XY}(0, 0) := \frac{1}{2} \text{Tr}[|0\rangle\langle 0| B N_{A \rightarrow B}(|0\rangle\langle 0| A)]$$  

(A19)

$$= \frac{1}{2} (1 - Q),$$  

(A20)
It is then straightforward to show that
\[ p_{XY}(0,1) := \frac{1}{2} \text{Tr}[|1\rangle(1)_B \mathcal{N}_{A \to B}(|0\rangle\langle 0|_A)] \] (A21)
\[ = \frac{1}{2} Q, \] (A22)
\[ p_{XY}(1,0) := \frac{1}{2} \text{Tr}[|0\rangle(0)_B \mathcal{N}_{A \to B}(|1\rangle\langle 1|_A)] \] (A23)
\[ = \frac{1}{2} Q, \] (A24)
\[ p_{XY}(1,1) := \frac{1}{2} \text{Tr}[|1\rangle(1)_B \mathcal{N}_{A \to B}(|1\rangle\langle 1|_A)] \] (A25)
\[ = \frac{1}{2} (1 - Q), \] (A26)
which is consistent with the probability distribution \( p_X \) in (129)–(132).

In general,
\[ p_{XY}(0,0) := \frac{1}{2} \text{Tr}[|0\rangle(0)_B \mathcal{N}_{A \to B}(|0\rangle\langle 0|_A)] \] (A27)
\[ = \frac{1}{2} (p_1 + p_2), \] (A28)
\[ p_{XY}(0,1) := \frac{1}{2} \text{Tr}[|1\rangle(1)_B \mathcal{N}_{A \to B}(|0\rangle\langle 0|_A)] \] (A29)
\[ = \frac{1}{2} (p_3 + p_4), \] (A30)
\[ p_{XY}(1,0) := \frac{1}{2} \text{Tr}[|0\rangle(0)_B \mathcal{N}_{A \to B}(|1\rangle\langle 1|_A)] \] (A31)
\[ = \frac{1}{2} (p_3 + p_4), \] (A32)
\[ p_{XY}(1,1) := \frac{1}{2} \text{Tr}[|1\rangle(1)_B \mathcal{N}_{A \to B}(|1\rangle\langle 1|_A)] \] (A33)
\[ = \frac{1}{2} (p_1 + p_2). \] (A34)

Then,
\[ \rho_{XY} = \frac{1}{2} (p_1 + p_2) |0\rangle\langle 0| + \frac{1}{2} (p_3 + p_4) |0\rangle\langle 1| \\
+ \frac{1}{2} (p_3 + p_4) |1\rangle\langle 0| \\
+ \frac{1}{2} (p_1 + p_2) |1\rangle\langle 1|. \] (A35)

It is then straightforward to show that
\[ I(X; Y) = 1 + p_1 + p_2 \log_2(p_1 + p_2) \\
+ p_3 + p_4 \log_2(p_3 + p_4). \] (A36)

where \( h_2 \) is the binary entropy function.

Let us now calculate \( V(X; Y)_\rho \). We have
\[ V(\rho||\sigma) := \text{Tr}[\rho \log_2 \rho - \log_2 \sigma] - D(\rho||\sigma)^2, \] (A38)
and
\[ V(X; Y)_\rho := V(\rho_{XY} \rho_X \rho_Y) \] (A39)
\[ = \text{Tr}[\rho_{XY}(\log_2 \rho_{XY} - \log_2(\rho_X \rho_Y))^2] - I(X; Y)_\rho. \] (A40)

One can show that
\[ \text{Tr}[\rho_{XY}(\log_2 \rho_{XY} - \log_2(\rho_X \rho_Y))^2] \\
= (p_1 + p_2) (1 + \log_2(p_1 + p_2))^2 \\
+ (p_3 + p_4) (1 + \log_2(p_3 + p_4))^2, \] (A41)
from which it follows that
\[ V(X; Y)_\rho = (p_1 + p_2) (p_3 + p_4) \left( \frac{\log_2 \left( \frac{p_1 + p_2}{p_3 + p_4} \right)}{p_3 + p_4} \right)^2. \] (A42)

We now calculate \( I(X; E) \) and \( V(X; E) \). We consider the following purification of the Choi state of the channel in (A1):
\[ |\psi\rangle_{ABE} := \sqrt{p_1} |\Phi^+\rangle_{AB} |0, 0\rangle_E + \sqrt{p_2} |\Phi^-\rangle_{AB} |1, 1\rangle_E \\
+ \sqrt{p_3} |\Psi^+\rangle_{AB} |0, 1\rangle_E + \sqrt{p_4} |\Psi^-\rangle_{AB} |1, 0\rangle_E. \] (A43)

Now,
\[ \langle 0|_A \otimes I_{BE} |\psi\rangle_{ABE} \\
= \langle 0|_B \frac{1}{\sqrt{2}} (\sqrt{p_1} |0, 0\rangle_E + \sqrt{p_2} |1, 1\rangle_E) \\
+ \langle 1|_B \frac{1}{\sqrt{2}} (\sqrt{p_3} |0, 1\rangle_E + \sqrt{p_4} |1, 0\rangle_E), \] (A44)
\[ \langle 1|_A \otimes I_{BE} |\psi\rangle_{ABE} \\
= \langle 1|_B \frac{1}{\sqrt{2}} (\sqrt{p_1} |0, 0\rangle_E - \sqrt{p_2} |1, 1\rangle_E) \\
+ \langle 0|_B \frac{1}{\sqrt{2}} (\sqrt{p_3} |0, 1\rangle_E - \sqrt{p_4} |1, 0\rangle_E). \] (A45)

Using this, we obtain
\[ \rho_{XE} = \frac{1}{2} |0\rangle\langle 0|_X \otimes \rho_{E|X=0} + \frac{1}{2} |1\rangle\langle 1|_X \otimes \rho_{E|X=1} \] (A46)
The state $\rho_{XE}$ can be diagonalized as follows:

$$
\rho_{XE} = \left(\frac{p_1 + p_2}{2}\right)|0\rangle\langle 0| \otimes |\Phi^+_{p_1, p_2}\rangle \langle \Phi^+_{p_1, p_2}| + \left(\frac{p_1 + p_2}{2}\right)|1\rangle\langle 1| \otimes |\Phi^-_{p_1, p_2}\rangle \langle \Phi^-_{p_1, p_2}| + \left(\frac{p_1 + p_4}{2}\right)|0\rangle\langle 0| \otimes |\Phi^+_{p_3, p_4}\rangle \langle \Phi^+_{p_3, p_4}| + \left(\frac{p_1 + p_4}{2}\right)|1\rangle\langle 1| \otimes |\Phi^-_{p_3, p_4}\rangle \langle \Phi^-_{p_3, p_4}|, \tag{A48}
$$

where

$$
|\Phi^\pm_{p_1, p_2} := \frac{1}{\sqrt{p_1 + p_2}} \left(\sqrt{\frac{p_1}{2}}|0, 0\rangle \pm \sqrt{\frac{p_2}{2}}|1, 1\rangle\right), \tag{A49}
$$

$$
|\Phi^\pm_{p_3, p_4} := \frac{1}{\sqrt{p_3 + p_4}} \left(\sqrt{\frac{p_3}{2}}|0, 1\rangle \pm \sqrt{\frac{p_4}{2}}|1, 0\rangle\right). \tag{A50}
$$

Then, by observing that

$$
\rho_E := \text{Tr}_X[\rho_{XE}] = p_1|0, 0\rangle\langle 0, 0| + p_3|0, 1\rangle\langle 0, 1| + p_4|1, 0\rangle\langle 1, 0| + p_2|1, 1\rangle\langle 1, 1|, \tag{A51}
$$

we find that

$$
I(X; E) = H(\bar{p}) - h_2(p_1 + p_2), \tag{A52}
$$

where

$$
H(\bar{p}) := \sum_{i=1}^4 -p_i \log_2 p_i. \tag{A53}
$$

Finally, for $V(X; E)$, it is straightforward to show that

$$
\text{Tr}[\rho_{XE}(\log_2 \rho_{XE} - \log_2(\rho_X \otimes \rho_E))^2] = p_1 \left(\log_2 \left(\frac{p_1}{p_1 + p_2}\right)\right)^2 + p_2 \left(\log_2 \left(\frac{p_2}{p_1 + p_2}\right)\right)^2
+ p_3 \left(\log_2 \left(\frac{p_3}{p_3 + p_4}\right)\right)^2 + p_4 \left(\log_2 \left(\frac{p_4}{p_3 + p_4}\right)\right)^2, \tag{A54}
$$

from which it follows that

$$
V(X; E) = p_1 \left(\log_2 \left(\frac{p_1}{p_1 + p_2}\right)\right)^2 + p_2 \left(\log_2 \left(\frac{p_2}{p_1 + p_2}\right)\right)^2 + p_3 \left(\log_2 \left(\frac{p_3}{p_3 + p_4}\right)\right)^2 + p_4 \left(\log_2 \left(\frac{p_4}{p_3 + p_4}\right)\right)^2 - (H(\bar{p}) - h_2(p_1 + p_2))^2. \tag{A55}
$$

For the six-state protocol, by using the formulas above and (A2)–(A4), we obtain

$$
I(X; Y)_\rho = 1 - h_2(Q), \tag{A56}
$$

$$
V(X; Y)_\rho = Q(1 - Q) \left(\log_2 \left(\frac{1 - Q}{Q}\right)\right)^2, \tag{A57}
$$

$$
I(X; E)_\rho = - \left(1 - \frac{3Q}{2}\right) \log_2 \left(\frac{1 - 3Q}{2}\right) - \frac{3Q}{2} \log_2 \left(\frac{Q}{2}\right) - h_2(Q), \tag{A58}
$$

$$
V(X; E)_\rho = Q + \left(1 - \frac{3Q}{2}\right) \log_2 \left(\frac{1 - \frac{3Q}{2}}{1 - Q}\right)^2 + \frac{Q}{2} \log_2 \left(\frac{\frac{Q}{2}}{1 - Q}\right)^2 - I(X; E)_\rho^2. \tag{A59}
$$

For the BB84 protocol, by using the formulas above and (A13)–(A18), we obtain

$$
I(X; Y)_\rho = 1 - h_2(Q), \tag{A60}
$$

$$
V(X; Y)_\rho = Q(1 - Q) \left(\log_2 \left(\frac{1 - Q}{Q}\right)\right)^2, \tag{A61}
$$

$$
I(X; E)_\rho = H(\{1 - 2Q + s, Q - s, Q - s, s\}) - h_2(Q), \tag{A62}
$$

$$
V(X; E)_\rho = (1 - 2Q + s) \left(\log_2 \left(\frac{1 - 2Q + s}{1 - Q}\right)\right)^2 + (Q - s) \log_2 \left(\frac{Q - s}{1 - Q}\right)^2 + (Q - s) \log_2 \left(\frac{Q - s}{Q}\right)^2. \tag{A63}
$$
\[ + s \left( \log_2 \left( \frac{s}{Q} \right) \right)^2 - I(X; E)_p. \quad \text{(A63)} \]

**Appendix B: Relation between smooth max-mutual informations**

Here we prove the following lemma relating two different variants of smooth max-mutual information:

**Lemma 7** Let \( \rho_{AE} \) be a bipartite state acting on a separable Hilbert space \( \mathcal{H}_A \otimes \mathcal{H}_E \), and let \( \varepsilon, \delta > 0 \) be such that \( \varepsilon + \delta < 1 \). Then

\[
\tilde{I}_{\varepsilon, \delta}^r(A; E)_p \leq D_{\text{max}}^r(\rho_{AE}\|\rho_A \otimes \rho_E) + \log_2 \left( \frac{8}{\delta^2} \right), \tag{B1} \]

where \( \tilde{I}_{\varepsilon, \delta}^r(A; E)_p \) is defined in (192) and \( D_{\text{max}}^r(\rho_{AE}\|\rho_A \otimes \rho_E) \) in (191).

**Proof.** The proof follows the proof of [ABJT18, Theorem 2], but has some differences because it is not necessary in our case to ensure partial smoothing. Let \( \tilde{\rho}_{AE} \) be a state satisfying \( P(\tilde{\rho}_{AE}, \rho_{AE}) \leq \varepsilon \). Let \( \gamma = \delta^2/8 \), and set \( \Pi_A^\gamma \) to be the projection onto the positive eigenspace of \( \frac{1}{\gamma} \rho_A - \rho_A \). Then it follows that

\[
\Pi_A^\gamma \left( \frac{1}{\gamma} \rho_A - \rho_A \right) \Pi_A^\gamma \geq 0
\]

\[
\Rightarrow \Pi_A^\gamma \rho_A \Pi_A^\gamma \leq \frac{1}{\gamma} \Pi_A^\gamma \tilde{\rho}_A \Pi_A^\gamma = \frac{8}{\delta^2} \Pi_A^\gamma \tilde{\rho}_A \Pi_A^\gamma, \tag{B2} \]

and

\[
(I - \Pi_A^\gamma) \left( \frac{1}{\gamma} \rho_A - \rho_A \right) (I - \Pi_A^\gamma) \leq 0
\]

\[
\Rightarrow \text{Tr}[(I - \Pi_A^\gamma) \tilde{\rho}_A] \leq \gamma \text{Tr}[(I - \Pi_A^\gamma) \rho_A] \leq \gamma = \frac{\delta^2}{8}, \tag{B3} \]

where the last inequality follows because \( \text{Tr}[(I - \Pi_A^\gamma) \rho_A] \leq 1 \). The inequality in (B3) can be rewritten as

\[
\text{Tr}[(I - \Pi_A^\gamma) \tilde{\rho}_A] \geq 1 - \frac{\delta^2}{8}. \tag{B4} \]

Let us define the following states:

\[
\rho_{AE}^{\text{EX}} := \Pi_A^\gamma \tilde{\rho}_{AE} \Pi_A^\gamma \otimes |0\rangle|0\rangle_X
\]

\[+ (I - \Pi_A^\gamma) \tilde{\rho}_{AE} (I - \Pi_A^\gamma) \otimes |1\rangle|1\rangle_X, \quad \text{(B5)} \]

\[
\tilde{\rho}_{AE}^{\text{EX}} := \left( \Pi_A^\gamma \tilde{\rho}_{AE} \Pi_A^\gamma + \tilde{\rho}_A^{1/2} (I - \Pi_A^\gamma) \tilde{\rho}_A^{1/2} \otimes \rho_E \right) \otimes |0\rangle|0\rangle_X, \quad \text{(B6)} \]

so that

\[
\tilde{\rho}_{AE} = \text{Tr}_X[\tilde{\rho}_{AE}^{\text{EX}}]
\]

\[
= \Pi_A^\gamma \tilde{\rho}_{AE} \Pi_A^\gamma + \tilde{\rho}_A^{1/2} (I - \Pi_A^\gamma) \tilde{\rho}_A^{1/2} \otimes \rho_E. \tag{B7} \]

Then, using the inequality \( \tilde{\rho}_{AE} \leq \mu \rho_A \otimes \rho_E \), with

\[
\mu := 2D_{\text{max}}(\tilde{\rho}_{AE}\|\rho_A \otimes \rho_E), \tag{B8} \]

and the fact that \( \mu \frac{8}{\delta^2} \geq 1 \) (which holds because \( D_{\text{max}}(\tilde{\rho}_{AE}\|\rho_A \otimes \rho_E) \geq 0 \) and \( \delta \geq 2^3 \)), we find that

\[
\tilde{\rho}_{AE} \leq \mu \Pi_A^\gamma \rho_A \Pi_A^\gamma \otimes \rho_E + \tilde{\rho}_A^{1/2} (I - \Pi_A^\gamma) \tilde{\rho}_A^{1/2} \otimes \rho_E
\]

\[
\leq \mu \frac{8}{\delta^2} \left[ \Pi_A^\gamma \tilde{\rho}_A \Pi_A^\gamma \otimes \rho_E + \tilde{\rho}_A^{1/2} (I - \Pi_A^\gamma) \tilde{\rho}_A^{1/2} \otimes \rho_E \right]
\]

\[
= \mu \frac{8}{\delta^2} \left[ \Pi_A^\gamma \tilde{\rho}_A \Pi_A^\gamma + \tilde{\rho}_A^{1/2} (I - \Pi_A^\gamma) \tilde{\rho}_A^{1/2} \right] \otimes \rho_E
\]

\[
= \frac{8}{\delta^2} \tilde{\rho}_A \otimes \rho_E. \tag{B9} \]

The second inequality above follows from (B2). Applying the definition of \( D_{\text{max}}(\tilde{\rho}_{AE}\|\rho_A \otimes \rho_E) \), we conclude that

\[
D_{\text{max}}(\tilde{\rho}_{AE}\|\rho_A \otimes \rho_E) \leq \tilde{D}_{\text{max}}(\tilde{\rho}_{AE}\|\rho_A \otimes \rho_E) + \log_2 \left( \frac{8}{\delta^2} \right). \tag{B11} \]

We can conclude the statement of the lemma if \( P(\tilde{\rho}_{AE}, \rho_{AE}) \leq \varepsilon + \delta \), and so it is our aim to show this now. Consider that

\[
P(\tilde{\rho}_{AE}^{\text{EX}}, \rho_{AE}^{\text{EX}}) = \sqrt{1 - F(\tilde{\rho}_{AE}^{\text{EX}}, \rho_{AE}^{\text{EX}})}. \tag{B12} \]

The following chain of inequalities holds

\[
\sqrt{F(\tilde{\rho}_{AE}^{\text{EX}}, \rho_{AE}^{\text{EX}})}
\]

\[
= \text{Tr} \left[ \left( \Pi_A^\gamma \tilde{\rho}_{AE} \Pi_A^\gamma \right) \left( \sqrt{\Pi_A^\gamma \tilde{\rho}_{AE} \Pi_A^\gamma} \left( \sqrt{\Pi_A^\gamma \tilde{\rho}_{AE} \Pi_A^\gamma} \right)^{1/2} \right) \right]^{1/2}
\]

\[
\geq \text{Tr} \left[ \left( \Pi_A^\gamma \tilde{\rho}_{AE} \Pi_A^\gamma \left( \sqrt{\Pi_A^\gamma \tilde{\rho}_{AE} \Pi_A^\gamma} \right)^{1/2} \right) \right]
\]

\[
= \text{Tr} \left[ \Pi_A^\gamma \tilde{\rho}_{AE} \Pi_A^\gamma \right]
\]

\[
= \text{Tr} \left[ \Pi_A^\gamma \tilde{\rho}_{AE} \Pi_A^\gamma \right]
\]

\[
\geq 1 - \frac{\delta^2}{8}, \tag{B13} \]

where the inequality follows from operator monotonicity of the square root and the fact that

\[
\tilde{\rho}_{AE} = \Pi_A^\gamma \tilde{\rho}_{AE} \Pi_A^\gamma + \tilde{\rho}_A^{1/2} (I - \Pi_A^\gamma) \tilde{\rho}_A^{1/2} \otimes \rho_E \tag{B14} \]

\[
\geq \Pi_A^\gamma \tilde{\rho}_{AE} \Pi_A^\gamma \tag{B15} \]

From the above and (B4), we conclude that

\[
F(\tilde{\rho}_{AE}^{\text{EX}}, \rho_{AE}^{\text{EX}}) \leq 1 - \frac{\delta^2}{4}, \tag{B16} \]

which implies that

\[
P(\tilde{\rho}_{AE}^{\text{EX}}, \rho_{AE}^{\text{EX}}) \leq \frac{\delta}{2}. \tag{B16} \]
Now consider that

\[
\begin{align*}
P(p_{AE}, p_{AE} \otimes |0\rangle\langle 0|_X) \\
\leq P(p_{AE}, p_{AE} \otimes |0\rangle\langle 0|_X) + P(\tilde{\rho}_{AE}, \rho_{AE}) \\
= \sqrt{1 - F(\tilde{\rho}_{AE}, \rho_{AE} \otimes |0\rangle\langle 0|_X)} + P(\tilde{\rho}_{AE}, \rho_{AE}) \\
= \sqrt{1 - \left(\sum A\tilde{\rho}_{AE} \sum A\tilde{\rho}_{AE} \sum A\tilde{\rho}_{AE} \sum A\tilde{\rho}_{AE}\right) + P(\tilde{\rho}_{AE}, \rho_{AE})} \\
= \sqrt{1 - \left(\sum A\tilde{\rho}_{AE} \sum A\tilde{\rho}_{AE} \sum A\tilde{\rho}_{AE} \sum A\tilde{\rho}_{AE}\right) + P(\tilde{\rho}_{AE}, \rho_{AE})} \\
\leq \frac{\delta}{2} + \varepsilon, \quad (B17)
\end{align*}
\]

where we applied the triangle inequality of the sine distance [Ras02, Ras03, Ras06, GLN05] for the first inequality and the fact that \(\|\sqrt{\Pi} = \sqrt{\Pi\Pi\sqrt{\tau} = \sqrt{\Pi\Pi\Pi\Pi\tau} = \sqrt{\Pi\Pi\Pi\Pi\tau}\|_1\) for a projector \(\Pi\) and states \(\omega\) and \(\tau\). Combining this with (B16), we find that

\[
\begin{align*}
P(\tilde{\rho}_{AE}, \rho_{AE}) \\
\leq P(\tilde{\rho}_{AE}, \rho_{AE} \otimes |0\rangle\langle 0|_X) \quad (B18) \\
\leq P(\tilde{\rho}_{AE}, \rho_{AE}) + P(\tilde{\rho}_{AE}, \rho_{AE} \otimes |0\rangle\langle 0|_X) \quad (B19) \\
= \varepsilon + \delta. \quad (B20)
\end{align*}
\]

Since we have found a state \(\tilde{\rho}_{AE}\) satisfying \(P(\tilde{\rho}_{AE}, \rho_{AE}) \leq \varepsilon + \delta\) and (B11), we conclude that

\[
\tilde{\tau}_{max}^\pm (E; A) \leq D_{max}(\tilde{\rho}_{AE} \rho_{AE}) + \log_2 \left(\frac{8}{\delta^2}\right). \quad (B21)
\]

Since this inequality has been shown for all states \(\tilde{\rho}_{AE}\) satisfying \(P(\tilde{\rho}_{AE}, \rho_{AE}) \leq \varepsilon\), we conclude the statement of the lemma.

### Appendix C: Smooth universal convex split lemma

for states acting on a separable Hilbert space

Here we prove a smooth universal convex split lemma for states acting on a separable Hilbert space:

**Lemma 8 (Smooth universal convex split)** Let \(S\) be a set, and let \(\rho^s_{AE}\) be a state acting on a separable Hilbert space \(H_A \otimes H_E\), such that \(\Tr_E(\rho^s_{AE}) = \rho_A\) for all \(s \in S\). Let \(\tau^s_{A_1 \cdots A_R E}\) denote the following state:

\[
\begin{align*}
\tau^s_{A_1 \cdots A_R E} := \\
\frac{1}{R} \sum_{r=1}^{R} \rho_{A_1} \otimes \cdots \otimes \rho_{A_{r-1}} \otimes \rho^s_{A_r E} \otimes \rho_{A_{r+1}} \otimes \cdots \otimes \rho_{A_R}. 
\end{align*}
\]

Let \(\varepsilon \in (0, 1)\) and \(\eta \in (0, \sqrt{\varepsilon})\). If

\[
\log_2 R \geq \sup_{s \in S} \tilde{F}^\pm - \eta^\pm (E; A)_{\rho^s} + 2\log_2 \left(\frac{1}{2\eta}\right), \quad (C2)
\]

then for all \(s \in S\), there exists a state \(\tilde{\rho}_{E}\) satisfying

\[
\frac{1}{2} \left\| \tau^s_{A_1 \cdots A_R E} - \rho_{A_1} \otimes \cdots \otimes \rho_{A_R} \otimes \tilde{\rho}_{E}\right\|_1 \leq \sqrt{\varepsilon}, \quad (C3)
\]

and \(P(\tilde{\rho}_{E}, \rho^s_{E}) \leq \sqrt{\varepsilon} - \eta\).

**Proof.** Fix \(s \in S\). Let \(\tilde{\rho}_{AE}\) be an arbitrary state satisfying \(P(\tilde{\rho}_{AE}, \rho^s_{AE}) \leq \sqrt{\varepsilon} - \eta\) and is such that

\[
\rho^s_A \otimes \tilde{\rho}_{E} = p\rho^s_{AE} + (1 - p) \omega^s_{AE}, \quad (C4)
\]

for some \(p \in (0, 1)\) and \(\omega^s_{AE}\) some state. We define the following state, which we think of as an approximation to \(\tau^s_{A_1 \cdots A_R E}\):

\[
\tau^s_{A_1 \cdots A_R E} := \\
\frac{1}{R} \sum_{r=1}^{R} \rho_{A_1} \otimes \cdots \otimes \rho_{A_{r-1}} \otimes \rho^s_{A_r E} \otimes \rho_{A_{r+1}} \otimes \cdots \otimes \rho_{A_R}. \quad (C5)
\]

It is a good approximation if \(\sqrt{\varepsilon} - \eta\) is small, because

\[
\sqrt{F}(\tau^s_{A_1 \cdots A_R E}, \tau_{A_1 \cdots A_R E}) \geq \frac{1}{R} \sum_{r=1}^{R} \sqrt{F}(\rho^s_A \otimes \cdots \otimes \rho_{A_{r-1}} \otimes \rho^s_{A_r E} \otimes \cdots \otimes \rho_{A_R}) \quad (C6)
\]

\[
= \frac{1}{R} \sum_{r=1}^{R} \sqrt{F}(\rho^s_{A_r E}, \rho^s_{A_r E}) \quad (C7)
\]

\[
= \sqrt{F}(\rho^s_{A_r E}, \rho^s_{A_r E}), \quad (C8)
\]

which in turn implies that

\[
\sqrt{F}(\tau^s_{A_1 \cdots A_R E}, \tau_{A_1 \cdots A_R E}) \geq \sqrt{F}(\rho^s_{A_r E}, \rho^s_{A_r E}). \quad (C9)
\]

So the inequality in (C9), the definition of the sine distance, and the fact that \(P(\tilde{\rho}_{AE}, \rho^s_{AE}) \leq \sqrt{\varepsilon} - \eta\) imply that

\[
P(\tau^s_{A_1 \cdots A_R E}, \tau_{A_1 \cdots A_R E}) \leq \sqrt{\varepsilon} - \eta, \quad (C10)
\]

and in turn that

\[
\frac{1}{2} \left\| \tau^s_{A_1 \cdots A_R E} - \tau_{A_1 \cdots A_R E}\right\|_1 \leq \sqrt{\varepsilon} - \eta. \quad (C11)
\]

Now, following [LW19, Appendix A] closely, let us define the following states:

\[
\beta^s_{AE} := \rho^s_A \otimes \tilde{\rho}_{E}, \quad (C12)
\]

\[
\alpha^s_{AE} := \tilde{\rho}_{AE}, \quad (C13)
\]
and observe that
\[
\text{Tr}_{E^R} ((\beta^{s}_{AE})^{\otimes R}) = \rho_A \otimes \cdots \otimes \rho_{AR} \otimes \tilde{\rho}_E^s,
\]
\[
\text{Tr}_{E^R} (\tilde{\tau}^R_{AE}) = \tilde{\tau}^R_{A_{1}} \cdots A_{R} E.
\]
Thus, it follows from data processing of normalized trace distance that
\[
\frac{1}{2} \left\| \tilde{\tau}^R_{A_{1}} \cdots A_{R} E - \rho_A \otimes \cdots \otimes \rho_{AR} \otimes \tilde{\rho}_E^s \right\|_1 
\leq \frac{1}{2} \left\| \tilde{\tau}^R_{AE} - (\beta^{s}_{AE})^{\otimes R} \right\|_1.
\]  

Now applying [LW19, Lemma 15], we find that
\[
\frac{1}{2} \left\| \tilde{\tau}^R_{A_{1}} \cdots A_{R} E - \rho_A \otimes \cdots \otimes \rho_{AR} \otimes \tilde{\rho}_E^s \right\|_1 \leq \eta
\]
if
\[
\log_2 R \geq \log_2 (1/p) + 2 \log_2 \left( \frac{1}{2\eta} \right).
\]

For the same choice of $R$, it follows from (17) that
\[
\frac{1}{2} \left\| \tilde{\tau}^R_{A_{1}} \cdots A_{R} E - \rho_A \otimes \cdots \otimes \rho_{AR} \otimes \tilde{\rho}_E^s \right\|_1 \leq \eta
\]
if
\[
\frac{1}{2} \left\| \tilde{\tau}^R_{A_{1}} \cdots A_{R} E - \rho_A \otimes \cdots \otimes \rho_{AR} \otimes \tilde{\rho}_E^s \right\|_1 \leq \sqrt{\varepsilon}.
\]

The whole argument above holds for an arbitrary state $\tilde{\rho}_{AE}$ satisfying $P(\rho_{AE}, \tilde{\rho}_{AE}) \leq \sqrt{\varepsilon} - \eta$ and (C4), and so taking an infimum of $\log_2 (1/p)$ over all states satisfying these conditions, and applying the definition in (192), as well as (187), we find that
\[
\frac{1}{2} \left\| \tilde{\tau}^R_{A_{1}} \cdots A_{R} E - \rho_A \otimes \cdots \otimes \rho_{AR} \otimes \tilde{\rho}_E^s \right\|_1 \leq \sqrt{\varepsilon}
\]
if
\[
\log_2 R \geq T^\varepsilon_{\max}(E; A)_{\rho^s} + 2 \log_2 \left( \frac{1}{2\eta} \right).
\]

Now note that the whole argument holds for all $s \in S$, due to the uniform structure of the convex split method, which consists of bringing in a tensor-power state and performing a random permutation. We then find that
\[
\frac{1}{2} \left\| \tilde{\tau}^R_{A_{1}} \cdots A_{R} E - \rho_A \otimes \cdots \otimes \rho_{AR} \otimes \tilde{\rho}_E^s \right\|_1 \leq \sqrt{\varepsilon}
\]
for all $s \in S$ if
\[
\log_2 R \geq \sup_{s \in S} T^\varepsilon_{\max}(E; A)_{\rho^s} + 2 \log_2 \left( \frac{1}{2\eta} \right).
\]
This concludes the proof. 

### Appendix D: Duality of smooth max-relative entropy

This appendix generalizes a duality relation for smooth max-relative entropy from the finite-dimensional case [JN12] to the case of states acting on a separable Hilbert space. Recall that the smooth max-relative entropy is defined as
\[
D^\varepsilon_{\max}(\rho||\sigma) = \log_2 \inf_{\tilde{\rho}} \inf_{\lambda \geq 0} \{ \lambda : \tilde{\rho} \leq \lambda \sigma \}.
\]

We can also define the dual smooth max-relative entropy as
\[
\tilde{D}^\varepsilon_{\max}(\rho||\sigma) := \log_2 \sup_{M \geq 0} \inf_{\tilde{\rho}, \lambda \leq \varepsilon} \{ \text{Tr}[M\tilde{\rho}] : \text{Tr}[M\sigma] \leq 1 \},
\]
where the supremum is with respect to all compact bounded operators $M \geq 0$, as these are dual to the trace-class operators [RS78]. In this section, for both of the above quantities, we expand the definitions to allow for subnormalized states $\rho$ and $\sigma$ (i.e., such that $\text{Tr}[\rho], \text{Tr}[\sigma] \leq 1$) and the sine distance becomes as follows [Tom15]:
\[
P(\tau, \omega) := \sqrt{1 - F(\tau \oplus (1 - \text{Tr}[\tau]), \omega \oplus (1 - \text{Tr}[\omega]))}.
\]

In what follows, we call subnormalized states “substates” for short. Note that for any projection $\Pi$ and substates $\tau$ and $\omega$, the following inequality holds [Tom15]
\[
P(\Pi\tau, \Pi\omega) \leq P(\tau, \omega).
\]

**Lemma 9** Let $\rho$ be a state and $\sigma$ a trace-class positive semi-definite operator acting on a separable Hilbert space $\mathcal{H}$. Let $\varepsilon \in (0, 1)$ and suppose that $D^\varepsilon_{\max}(\rho||\sigma) < \infty$. Then
\[
D^\varepsilon_{\max}(\rho||\sigma) = \tilde{D}^\varepsilon_{\max}(\rho||\sigma).
\]

**Proof.** We prove this in several steps, with the proof bearing some similarities to the approach from [FAR11, Appendix B] (see also [WW18, Appendix A] in this context). First, for a state $\tilde{\rho}$, consider from weak duality that
\[
\inf_{\lambda \geq 0} \{ \lambda : \tilde{\rho} \leq \lambda \sigma \} \sup_{M \geq 0} \{ \text{Tr}[M\tilde{\rho}] : \text{Tr}[M\sigma] \leq 1 \},
\]
where the optimization on the right-hand side is over the compact bounded operators, given that these are dual to the trace-class operators [RS78]. In more detail, let $\lambda \geq 0$ satisfy $\tilde{\rho} \leq \lambda \sigma$, and let $M$ be an arbitrary compact bounded operator satisfying $M \geq 0$ and $\text{Tr}[M\sigma] \leq 1$. Then it follows that $\lambda \geq \lambda \text{Tr}[M\tilde{\rho}]$, where we used $\tilde{\rho} \leq \lambda \sigma$ and $M \geq 0$. Since this inequality holds for all $\lambda$ and $M$ satisfying the given conditions, we conclude the weak duality inequality in (D6). Then we have that
\[
D^\varepsilon_{\max}(\rho||\sigma)
\]
\begin{align}
&= \log_2 \inf_{\tilde{\rho} : P(\tilde{\rho}, \rho) \leq \varepsilon} \inf \{ \lambda : \tilde{\rho} \leq \lambda \sigma \} \\
&\geq \log_2 \inf_{\tilde{\rho} : P(\tilde{\rho}, \rho) \leq \varepsilon} \sup_{M \geq 0} \{ \text{Tr}[M \tilde{\rho}] : \text{Tr}[M \sigma] \leq 1 \} \\
&\geq \log_2 \sup_{M \geq 0} \inf_{\tilde{\rho} : P(\tilde{\rho}, \rho) \leq \varepsilon} \{ \text{Tr}[M \tilde{\rho}] : \text{Tr}[M \sigma] \leq 1 \} \\
&= \tilde{D}_\varepsilon(\rho \| \sigma). 
\end{align}

So the following weak-duality inequality holds

\begin{equation}
D^\varepsilon_{\max}(\rho \| \sigma) \geq \tilde{D}_\varepsilon(\rho \| \sigma).
\end{equation}

Let \( \{ \Pi^k \} \) be a sequence of projectors onto finite-dimensional subspaces strongly converging to the identity operator, and suppose that \( \Pi^k \leq \Pi^{k'} \) for \( k \leq k' \). Then define

\begin{align}
\rho^k &\coloneqq \Pi^k \rho \Pi^k, \\
\sigma^k &\coloneqq \Pi^k \sigma \Pi^k.
\end{align}

We now prove that

\begin{equation}
\lim_{k \to \infty} D^\varepsilon_{\max}(\rho^k \| \sigma^k) = D^\varepsilon_{\max}(\rho \| \sigma).
\end{equation}

Let \( \tilde{\rho} \) be an arbitrary state satisfying \( P(\tilde{\rho}, \rho) \leq \varepsilon \) and let \( \lambda \) satisfy \( \tilde{\rho} \leq \lambda \sigma \). Then it follows that

\begin{align}
\rho^k &\coloneqq \Pi^k \rho \Pi^k \leq \lambda \Pi^k \sigma \Pi^k = \lambda \sigma^k, \\
P(\rho^k, \rho^k) &\leq \varepsilon,
\end{align}

so that

\begin{equation}
D^\varepsilon_{\max}(\rho^k \| \sigma^k) \leq \log_2 \lambda.
\end{equation}

Since \( \lambda \) and \( \tilde{\rho} \) are arbitrary, we conclude that

\begin{equation}
D^\varepsilon_{\max}(\rho^k \| \sigma^k) \leq D^\varepsilon_{\max}(\rho \| \sigma),
\end{equation}

and since this inequality holds for all \( k \), the following inequality holds

\begin{equation}
\limsup_{k \to \infty} D^\varepsilon_{\max}(\rho^k \| \sigma^k) \leq D^\varepsilon_{\max}(\rho \| \sigma).
\end{equation}

To show the opposite inequality, we first prove that \( D^\varepsilon_{\max}(\rho^k \| \sigma^k) \) is monotone non-decreasing with \( k \). (The proof is in fact similar to what we have just shown.) Fix \( k \) and \( k' \) such that \( k \leq k' \). Let \( \tilde{\rho}^{k'} \) be a state satisfying \( P(\tilde{\rho}^{k'}, \rho^{k'}) \leq \varepsilon \) and let \( \lambda^{k'} \) be such that \( \tilde{\rho}^{k'} \leq \lambda^{k'} \sigma^{k'} \). Then it follows that

\begin{equation}
\rho^{k', k} \coloneqq \Pi^k \tilde{\rho}^{k'} \Pi^k \leq \lambda^k \Pi^k \sigma^{k'} \Pi^k = \lambda^k \lambda^{k'} \sigma^{k},
\end{equation}

and

\begin{equation}
P(\rho^{k', k}, \Pi^k \rho^{k'} \Pi^k) = P(\rho^{k', k}, \rho^{k'}) \leq \varepsilon,
\end{equation}

so that

\begin{equation}
D^\varepsilon_{\max}(\rho^k \| \sigma^k) \leq \log_2 \lambda^{k'}.
\end{equation}

Since \( \lambda^{k'} \) and \( \tilde{\rho}^{k'} \) are arbitrary, it follows that

\begin{equation}
D^\varepsilon_{\max}(\rho^k \| \sigma^k) \leq D^\varepsilon_{\max}(\rho^{k'} \| \sigma^{k'}).
\end{equation}

Now let \( \rho^k \) and \( \lambda^k \) be the optimal state and value for \( D^\varepsilon_{\max}(\rho^k \| \sigma^k) \), so that \( \lambda^k = D^\varepsilon_{\max}(\rho^k \| \sigma^k) \). By what we have just shown, the sequence \( \lambda^k \) is monotone non-decreasing, and so the limit \( \lambda := \lim_{k \to \infty} \lambda^k \) is well defined. Also, we know from (D18) that \( \lambda \leq D^\varepsilon_{\max}(\rho \| \sigma) < \infty \). Due to the fact that \( \| \rho^k \|_1 = \text{Tr}[\rho^k] \leq \lambda^k \text{Tr}[\sigma^k] \leq \lambda \text{Tr}[\sigma] \), it follows that \( \rho^k \) is a bounded sequence in the trace-class operators. Since the trace-class operators form the dual space of the compact bounded operators [RS78], we apply the Banach–Alaoglu theorem [RS78] to find a subsequence \( \{ \rho^{k}_j \}_{j \in S} \) having a weak* limit \( \tilde{\rho} \), which means that \( \text{Tr}[K \tilde{\rho}^{k}_j] \to \text{Tr}[K \tilde{\rho}] \) for \( k \in S \) and for all compact bounded operators \( K \). It holds that \( \tilde{\rho} \) is positive semi-definite. Then it follows that \( \lambda^k \rho^k - \tilde{\rho} \) converges in the weak operator topology to \( \lambda \sigma - \tilde{\rho} \). Then we conclude that \( \lambda \sigma - \tilde{\rho} \geq 0 \), and finally that \( D^\varepsilon_{\max}(\rho \| \sigma) \leq \lambda \). So we conclude (D13).

By strong duality, and the fact that \( \rho^k \) and \( \sigma^k \) are finite-dimensional, it follows from [JN12] that

\begin{equation}
D^\varepsilon_{\max}(\rho^k \| \sigma^k) = \tilde{D}_\varepsilon(\rho^k \| \sigma^k)
\end{equation}

for all \( k \). So these equalities and (D13) imply that

\begin{equation}
\lim_{k \to \infty} \tilde{D}_\varepsilon(\rho^k \| \sigma^k) = D^\varepsilon_{\max}(\rho \| \sigma).
\end{equation}

Now our goal is to prove that

\begin{equation}
\lim_{k \to \infty} \tilde{D}_\varepsilon(\rho^k \| \sigma^k) \leq \tilde{D}_\varepsilon(\rho \| \sigma),
\end{equation}

and we adopt a similar approach as above for doing so. Let \( M^k \) be an arbitrary compact bounded operator satisfying \( \text{Tr}[M^k \sigma^k] \leq 1 \) and let \( \tilde{\rho} \) be an arbitrary state satisfying \( P(\tilde{\rho}, \rho) \leq \varepsilon \). Define \( \rho^k = \Pi^k \tilde{\rho}^k \tilde{\rho}^k \). Then it follows that

\begin{align}
\text{Tr}[M^k \sigma^k] = &\text{Tr}[\Pi^k M^k \Pi^k \sigma^k] \leq 1, \\
P(\tilde{\rho}^k, \rho^k) &\leq \varepsilon,
\end{align}

and

\begin{align}
&\inf_{\tilde{\rho}^k : P(\tilde{\rho}^k, \rho^k) \leq \varepsilon} \text{Tr}[M^k \tilde{\rho}^k] \leq \text{Tr}[M^k \tilde{\rho}^k]
\end{align}

\begin{align}
= &\text{Tr}[M^k \Pi^k \tilde{\rho}^k]
\end{align}

\begin{align}
= &\text{Tr}[\Pi^k M^k \tilde{\rho}^k]
\end{align}

Since the inequality holds for all \( \rho \) satisfying \( P(\tilde{\rho}, \rho) \leq \varepsilon \), we conclude that

\begin{align}
&\inf_{\tilde{\rho}^k : P(\tilde{\rho}^k, \rho^k) \leq \varepsilon} \text{Tr}[M^k \tilde{\rho}^k]
\end{align}

\begin{align}
\leq &\inf_{\tilde{\rho} : P(\tilde{\rho}, \rho) \leq \varepsilon} \text{Tr}[\Pi^k M^k \tilde{\rho}]
\end{align}

\begin{align}
\leq &\sup_{M_0 \geq 0 : P(\tilde{\rho}, \rho) \leq \varepsilon} \{ \text{Tr}[M_0 \tilde{\rho}] : \text{Tr}[M \sigma] \leq 1 \}
\end{align}

\begin{align}
= &\tilde{D}_\varepsilon(\rho \| \sigma),
\end{align}

where the second inequality follows because \( \Pi^k M^k \Pi^k \) is a particular compact bounded operator satisfying
Tr[Π^k M^k σ^k] ≤ 1. Since the inequality above has been shown for an arbitrary compact bounded operator $M^k$ satisfying $Tr[M^k σ^k] ≤ 1$, we conclude that

$$\sup_{M^k \geq 0} \inf_{\rho^k, P(\rho^k) \leq \epsilon} \{Tr[M^k \rho^k] : Tr[M^k σ^k] \leq 1\} = \hat{D}_0(\delta) := \hat{D}_0(\delta).$$

(D34)

Since this inequality has been shown for arbitrary $k$, we conclude that

$$\limsup_{k \to \infty} \hat{D}_0(\delta) \leq \hat{D}_0(\delta).$$

(D35)

Finally, by combining (D11), (D24), and (D25), we conclude that

$$\hat{D}_0(\delta) = D(\delta).$$

(D36)

This completes the proof. ■

Appendix E: Relation between smooth max-relative entropy and hypothesis testing relative entropy

This appendix establishes inequalities relating the smooth max-relative entropy and the hypothesis testing relative entropy of states acting on a separable Hilbert space.

Lemma 10 Let $\rho$ be a state and $\sigma$ a trace-class positive semi-definite operator acting on a separable Hilbert space $H$. Let $\epsilon \in (0, 1)$, and set $\delta \in (0, 1)$ such that $\epsilon + \delta < 1$. Suppose that $D^{\epsilon, \delta}(\rho, \sigma) < \infty$. Then the following bounds hold

$$D^{\epsilon, \delta}(\rho, \sigma) \leq \hat{D}_0(\delta) + \log(\frac{1 - \epsilon}{\epsilon}).$$

(E1)

$$D^{\epsilon, \delta}(\rho, \sigma) \leq D(\delta) + \log(\frac{1 - \epsilon}{\epsilon}).$$

(E2)

Proof. These bounds were established for the finite-dimensional case in [ABJT19, Theorem 4]. Here we check that the arguments presented in the proof of [ABJT19, Theorem 4] hold for the more general case in the statement of the lemma, and we combine with the result from Lemma 9.

We first consider the inequality in (E1). Let $M \geq 0$ be an arbitrary compact bounded operator satisfying $Tr[M \sigma] \leq 1$. Since $M$ is compact, it has a countable spectral decomposition as $M = \sum m_i \langle \phi_i | \phi_i \rangle$, where $\{m_i\}$ is a countable set of non-negative eigenvalues and $\{\langle \phi_i \rangle\}$ is a countable orthonormal basis. We define a measurement (or completely dephasing) channel as

$$\mathcal{M}(\cdot) := \sum_i |\phi_i \rangle \langle \phi_i | \langle \phi_i | \phi_i \rangle,$$

and we set the probability distributions $P$ and $Q$ such that

$$\mathcal{M}(\rho) = \sum_i P(i) |\phi_i \rangle \langle \phi_i |$$

and

$$\mathcal{M}(Q) = \sum_i Q(i) |\phi_i \rangle \langle \phi_i |.$$

(E3)

(E4)

Then the data processing inequality for the hypothesis testing relative entropy implies that

$$D^{\epsilon, \delta}(\rho, \sigma) \geq D^{\epsilon, \delta}(\rho, \sigma) \geq D^{\epsilon, \delta}(\rho, \sigma) := K,$$

(E6)

where the $\epsilon$-information spectrum for states $\tau$ and $\omega$ is defined as [TH13]

$$D^{\epsilon}(\tau, \omega) := \sup\{\lambda \in \mathbb{R} : Tr[\tau \{\tau \leq 2^\lambda \omega\}] \leq \epsilon\},$$

(E7)

and $\{\tau \leq 2^\lambda \omega\}$ denotes the projection onto the positive part of $2^\lambda \omega - \tau$. The second inequality above follows by picking $\Lambda := \{\tau > 2^\lambda \omega\}$ for $\lambda = D^{\epsilon}(\tau, \omega) - \xi$ and $\xi > 0$. Since $\Lambda$ satisfies $Tr[\Lambda \gamma] \geq 1 - \epsilon$, and we also have that

$$Tr[\Lambda \gamma] = \frac{\sum_{i \in I} Q(i) < 2^\lambda \rho}{K},$$

(E8)

it follows from definitions that

$$\lambda = D^{\epsilon}(\tau, \omega) - \xi \leq D^{\epsilon}(\tau, \omega).$$

(E11)

Since the inequality has been shown for all $\xi > 0$, it follows that $D^{\epsilon}(\tau, \omega) \leq D^{\epsilon}(\tau, \omega)$. Now set $\eta > 0$, and define the set

$$I := \{i : P(i) < 2^\eta Q(i)\},$$

(E12)

which implies that $P(I) := \sum_{i \in I} P(i) > 1 - \epsilon$ from the definition of $D^{\epsilon}(\tau, \omega)$ (indeed, from the definition of $D^{\epsilon}(\tau, \omega)$, $K$ is the largest possible value such that $\sum_{i \in I} P(i) \leq 1 - \epsilon$, so that if it is increased by $\eta > 0$, then $P(I) > 1 - \epsilon$). Now define the projection $\Pi := \sum_{i \in I} |\phi_i \rangle \langle \phi_i |$. Then it follows that

$$Tr[\Pi \rho] = Tr[\mathcal{M}(\Pi) \rho]$$

(E13)

$$= Tr[\Pi \mathcal{M}(\rho)]$$

(E14)

$$= 1 - P(I)$$

(E15)

$$\leq \epsilon.$$  

(E16)

Set

$$\bar{\rho} := \frac{(I - \Pi) \rho (I - \Pi)}{1 - Tr[\Pi \rho]}.$$ 

(E17)

Then it follows that $P(\rho, \bar{\rho}) \leq \sqrt{\epsilon}$ because

$$F(\rho, \bar{\rho}) = \frac{\sqrt{\bar{\rho}}}{\sqrt{\bar{\rho}}} = \frac{1}{1 - Tr[\Pi \rho]} \frac{\sqrt{\rho} \sqrt{(I - \Pi) \rho (I - \Pi)}}{1 - Tr[\Pi \rho]}$$

(E18)

$$= \frac{1}{1 - Tr[\Pi \rho]} \frac{\sqrt{\rho} \sqrt{(I - \Pi) \rho (I - \Pi)}}{1 - Tr[\Pi \rho]}$$

(E19)

$$= \frac{1}{1 - Tr[\Pi \rho]} \times$$
Consider an arbitrary operator \( \Lambda \) satisfying \( 0 \leq \Lambda \leq I \) and \( \text{Tr}[(I - \Lambda) \rho] = 1 - \varepsilon - \delta \). Then the data processing inequality for the fidelity, with respect to the measurement \( \{ \Lambda, I - \Lambda \} \), implies that
\[
\sqrt{1 - \varepsilon}
\]
\[\leq \sqrt{F(\rho, \psi)} = \sqrt{\text{Tr}[\Lambda \rho] \text{Tr}[\Lambda \rho] + \text{Tr}[(I - \Lambda) \rho] \text{Tr}[(I - \Lambda) \rho]}
\]
\[\leq 2^{\lambda} \sqrt{\text{Tr}[(I - \Lambda) \rho]} + 1 - \varepsilon - \delta.
\] (E34)

Now taking an infimum over all \( \lambda \) such that (E33) holds and all \( \Lambda \) satisfying \( 0 \leq \Lambda \leq I \) and \( \text{Tr}[(I - \Lambda) \rho] = 1 - \varepsilon - \delta \), and applying definitions, we find that
\[
\sqrt{1 - \varepsilon} \leq 2^{D_{\max}^2(\sigma || \sigma) - D_{\max}^H(\sigma || \sigma) + 1 - \varepsilon - \delta}.
\] (E35)

Rewriting this gives
\[
\log_2 \left( \sqrt{1 - \varepsilon} - \sqrt{1 - \varepsilon - \delta} \right)^2 \leq D_{\max}^2(\sigma || \sigma) - D_{\max}^H(\sigma || \sigma).
\] (E36)

Now applying the inequality \( \sqrt{1 - \varepsilon} - \sqrt{1 - \varepsilon - \delta} \geq \frac{\delta}{2\sqrt{1 - \varepsilon}} \), we conclude (E2).

**Appendix F: Second-order asymptotics of smooth max-relative entropy for states acting on a separable Hilbert space**

Recall the quantities defined in (247)–(249). We also define
\[
\Phi(a) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{a} dx \, \exp \left( -\frac{x^2}{2} \right),
\] (F1)
\[
\Phi^{-1}(\varepsilon) := \sup \{ a \in \mathbb{R} \mid \Phi(a) \leq \varepsilon \}.
\] (F2)

For \( \varepsilon \in (0, 1) \), observe that
\[
\Phi^{-1}(1 - \varepsilon) = -\Phi^{-1}(\varepsilon).
\] (F3)

Let us define the quantity \( T(\sigma || \sigma) \) \([\text{TH13, Li14, KW17}]\) as
\[
T(\sigma || \sigma) := \sum_{x,y} |\langle \phi_x | \psi_x \rangle|^2 \lambda_x \left| \log_2 \left( \frac{\lambda_x}{\mu_y} \right) - D(\sigma || \sigma) \right|^3
\] (F4)

where the eigendecompositions of the state \( \rho \) and the trace-class positive-semidefinite operator \( \sigma \) are given in (247). Then the following expansion holds for \( \rho, \sigma \) such that \( D(\sigma || \sigma), V(\rho || \sigma), T(\rho || \sigma) < \infty \) and \( V(\sigma || \rho) > 0 \):
\[
\frac{1}{n} D_{\max}^H(\rho || \sigma)^n = D(\rho || \sigma) + \sqrt{\frac{1}{n} V(\rho || \sigma) \Phi^{-1}(\varepsilon)} + O\left( \frac{\log n}{n} \right).
\] (F5)
The term $O\left(\frac{\log n}{n}\right)$ above hides constants involving $V(\rho\|\sigma)$, $T(\rho\|\sigma)$, and $\varepsilon$.

By combining the equality in (F5) with Lemma 10, we arrive at the following corollary, giving the second-order asymptotics for smooth max-relative entropy of trace-class operators acting on a separable Hilbert space:

**Corollary 11** Let $\varepsilon \in (0, 1)$. Let $\rho$ be a state and $\sigma$ a trace-class positive semi-definite operator acting on a separable Hilbert space $\mathcal{H}$, such that $D(\rho\|\sigma), V(\rho\|\sigma), T(\rho\|\sigma) < \infty$ and $V(\rho\|\sigma) > 0$. Then the following second-order expansion holds for sufficiently large $n$:

$$
\frac{1}{n} D^\varepsilon_{\max}(\rho^\otimes n\|\sigma^\otimes n) = \left[D(\rho\|\sigma) - \sqrt{\frac{1}{n} V(\rho\|\sigma) \Phi^{-1}(\varepsilon)} + O\left(\frac{\log n}{n}\right)\right].
$$

**Proof.** Exploiting the inequality in (E1), we find that

$$
\frac{1}{n} D^\varepsilon_{\max}(\rho^\otimes n\|\sigma^\otimes n) \leq \frac{1}{n} D^\varepsilon_{H}(\rho^\otimes n\|\rho^\otimes n) + \frac{1}{n} \log_2 \left(1 - \varepsilon\right) + \frac{1}{n} D(\rho\|\sigma) + \sqrt{\frac{1}{n} V(\rho\|\sigma) \Phi^{-1}(1 - \varepsilon)} + O\left(\frac{\log n}{n}\right)
$$

where the first equality follows from (F5) and the last equality follows from (F3). Now exploiting the inequality in (E2) and choosing $\delta = 1/\sqrt{n}$, we find that

$$
\frac{1}{n} D^\varepsilon_{\max}(\rho^\otimes n\|\sigma^\otimes n) \geq \frac{1}{n} D^\varepsilon_{H}(\rho^\otimes n\|\rho^\otimes n) - \frac{1}{n} \log_2 \left(\frac{4(1 - \varepsilon)}{\delta^2}\right)
$$

where the first equality follows from [TH13, Footnote 6] applied to $\Phi^{-1}(1 - \varepsilon - \delta)$, which is an invocation of Taylor’s theorem: for $f$ continuously differentiable, $c$ a positive constant, and $n \geq n_0$, the following equality holds

$$
\sqrt{n}f(x + c/\sqrt{n}) = \sqrt{n}f(x) + cf'(a)
$$

for some $a \in [x, x + c/\sqrt{n_0}]$. This concludes the proof. ■

---

**Appendix G: Mutual information variance and $T$ quantity of classical–quantum states**

**Proposition 12** Given is a classical–quantum state of the following form:

$$
\rho_{XB} := \sum_x p_X(x) |x\rangle\langle x| \otimes \rho_B^x.
$$

Suppose that $\rho_B^x$ and $\rho_B := \sum_x p_X(x) \rho_B^x$ have the following spectral decompositions:

$$
\rho_B^x = \sum_y p(y|x) |\psi^{x,y}\rangle\langle \psi^{x,y}|_B,
$$

$$
\rho_B = \sum_z q(z) |\phi^{z}\rangle\langle \phi^{z}|_B,
$$

where $p(y|x)$ a conditional probability distribution, $\{|\psi^{x,y}\rangle_B\}_y$ an orthonormal set of eigenvectors (for fixed $x$), $q(z)$ a probability distribution, and $\{|\phi^{z}\rangle_B\}_z$ an orthonormal set of eigenvectors. Then

$$
V(X; B)_\rho = \sum_x p_X(x) \left[ V(\rho_B^x\|\rho_B) + |D(\rho_B^x\|\rho_B)|^2 \right] - |I(X; B)|^2,
$$

$$
T(X; B)_\rho = \sum_x p_X(x) \sum_{y,z} |\langle \psi^{x,y}\|\phi^{z}\rangle_B|^2 p(y|x) |f(x, y, z)|^2,
$$

where

$$
f(x, y, z) := \log_2 (p(y|x)q(z)) - I(X; B).
$$

**Proof.** To see the first expression in (G4), consider that

$$
\log_2 \rho_{XB} - \log_2 \rho_X \otimes \rho_B
$$

$$
= \log_2 \left[ \sum_x |x\rangle\langle x| \otimes p_X(x) \rho_B^x \right]
$$

$$
= \log_2 \left[ \sum_x |x\rangle\langle x| \otimes \left( \log_2 \left[ p_X(x) \rho_B^x \right] - \log_2 \left[ p_X(x) \rho_B \right] \right) \right]
$$

$$
= \sum_x |x\rangle\langle x| \otimes \left( \log_2 \rho_B^x - \log_2 \rho_B \right),
$$

and we find that

$$
\left[ \log_2 \rho_{XB} - \log_2 \rho_X \otimes \rho_B - I(X; B) \right]^2
$$

$$
= \sum_x |x\rangle\langle x| \otimes \left( \log_2 \rho_B^x - \log_2 \rho_B - I(X; B) \right)^2,
$$

as desired.
so that
\[
\text{Tr}[\rho_{XX} (\log_2 \rho_{XX} - \log_2 \rho_X \otimes \rho_B - I(X;B))^2] = \text{Tr} \left[ \left( \sum_{x'} p_X(x') |x'\rangle \langle x' | \otimes \rho_B^{x'} \right) \times \left( \sum_{x} |x\rangle \langle x | \otimes (\log_2 \rho_B^{x} - \log_2 \rho_B - I(X;B))^2 \right) \right]
\]
\[
= \sum_{x} p_X(x) \text{Tr}[\rho_B^{x} (\log_2 \rho_B^{x} - \log_2 \rho_B - I(X;B))^2] = \sum_{x} p_X(x) \text{Tr}[\rho_B^{x} (\log_2 \rho_B^{x} - \log_2 \rho_B - I(X;B))^2] = \sum_{x} p_X(x) \text{Tr}[\rho_B^{x} (\log_2 \rho_B^{x} - \log_2 \rho_B - I(X;B))^2] - [I(X;B)]^2.
\]
\[
\text{(G10)}
\]
Now consider that
\[
\text{Tr}[\rho_B^{x} (\log_2 \rho_B^{x} - \log_2 \rho_B - I(X;B))^2] = \text{Tr}[\rho_B^{x} (\log_2 \rho_B^{x} - \log_2 \rho_B - I(X;B))^2] - [D(\rho_B^{x}\Vert \rho_B)]^2 + [D(\rho_B^{x}\Vert \rho_B)]^2 = [V(\rho_B^{x}\Vert \rho_B) + [D(\rho_B^{x}\Vert \rho_B)]^2].
\]
\[
\text{(G11)}
\]
Substituting the last line back in (G10) gives the formula in (G4).

To see the other expressions, consider that
\[
T(\rho_{XX} \Vert \rho_X \otimes \rho_B) = \sum_{x,x',y,z} \left[ \left( \langle x \rangle X \otimes \langle x' \rangle X \otimes \langle \phi \rangle B \right) \left( p(x) p(y|x) \langle \phi \rangle B \right) \left( \log_2 (p(x) p(y|x) \langle \phi \rangle B) \right) \left( I(X;B) \right) \right]^{3}
\]
\[
= \sum_{x,x',y,z} \left[ \left( p(x) p(y|x) \langle \phi \rangle B \right) \left( \log_2 (p(x) p(y|x) \langle \phi \rangle B) \right) \right]^{3}
\]
\[
\text{(G12)}
\]
and
\[
= \sum_{x} p(x) \sum_{y,z} \left[ \left( p(x) p(y|x) \langle \phi \rangle B \right) \left( \log_2 (p(x) p(y|x) \langle \phi \rangle B) \right) \right]^{3}
\]
\[
\text{(G13)}
\]
By employing a similar development as above, the formula in (G5) is then clear. 

### Appendix H: Holevo information and Holevo information variance of a Gaussian ensemble of Gaussian states

In what follows, we determine formulas for the Holevo information and Holevo information variance of a Gaussian ensemble of Gaussian states. The first is well known, but the expression we give for it seems to be novel. The latter has not been presented yet to our knowledge. Before presenting the formulas, we provide a brief review of quantum Gaussian states in order to set some notation. We refer to [Ser17] for an in-depth overview of quantum Gaussian states and measurements.

We consider m-mode Gaussian states, where m is some fixed positive integer. Let \( \hat{r} \) denote each quadrature operator (2m of them for an m-mode state), and let
\[
\hat{r} = \left[ \hat{x}_1, \hat{p}_1, \ldots, \hat{x}_m, \hat{p}_m \right]
\]
\[
\text{(H1)}
\]
denote the vector of quadrature operators, so that the odd entries correspond to position-quadrature operators and the even entries to momentum-quadrature operators. The quadrature operators satisfy the following commutation relations:
\[
[\hat{r}_j, \hat{r}_k] = i\Omega_{j,k}, \quad \text{where} \quad \Omega := I_m \otimes \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \text{(H3)}
\]
and \( I_m \) is the m \times m identity matrix. We also take the annihilation operator \( \hat{a} = (\hat{x} + i\hat{p})/\sqrt{2} \).

Let \( \rho \) be a Gaussian state, with the mean-vector entries
\[
\mu_j := \langle \hat{r}_j \rangle_{\rho}, \quad \text{(H4)}
\]
and let \( \mu \) denote the mean vector. The entries of the covariance matrix \( V \) of \( \rho \) are given by
\[
V_{j,k} \equiv \langle \{\hat{r}_j - \mu_j, \hat{r}_k - \mu_k\} \rangle_{\rho}, \quad \text{(H5)}
\]
and they satisfy the uncertainty principle \( V + i\Omega \geq 0 \). A 2m \times 2m matrix \( S \) is symplectic if it preserves the symplectic form: \( S\Omega S^T = \Omega \). According to Williamson's theorem [Wil36], there is a diagonalization of the covariance matrix \( V \) of the form,
\[
V = S (D \otimes I_2) S^T, \quad \text{(H6)}
\]
where \( S \) is a symplectic matrix and \( D \equiv \text{diag}(\nu_1, \ldots, \nu_m) \) is a diagonal matrix of symplectic eigenvalues such that \( \nu_i \geq 1 \) for all \( i \in \{1, \ldots, m\} \). We say that a quantum Gaussian state is faithful if all of its symplectic eigenvalues are strictly greater than one (this also means that the state is positive definite). We can write the density operator \( \rho \) of a faithful state in the following exponential form [Che05, Kru06, Hol10] (see also [Hol12, Ser17]):
\[
\rho = Z^{-1/2} \exp \left[ -\frac{1}{2} (\hat{r} - \mu)^T G (\hat{r} - \mu) \right], \quad \text{(H7)}
\]
with \( Z := \det([V + i\Omega]/2) \) and \( G := -2\Omega S [\arcoth(D) \otimes I_2] S^T \Omega \).
\[
\text{(H8)}
\]
where \( \arcoth(x) \equiv \frac{1}{2} \ln \left( \frac{x + 1}{x - 1} \right) \) with domain \(( -\infty, -1) \cup (1, +\infty) \). The matrix \( G \) is known as the Hamiltonian matrix [Ser17]. Note that we can also write
\[
G = 2\Omega \arcoth(iV\Omega), \quad \text{(H9)}
\]
so that \( G \) is represented directly in terms of the covariance matrix \( V \). Faithfulness of Gaussian states is required to ensure that \( G \) is non-singular. By inspection, the Hamiltonian matrix \( G \) and the covariance matrix \( V \) are symmetric.

Let \( \mu^p, V^p, G^p, Z^p \) denote the various quantities above for an m-mode quantum Gaussian state \( \rho \), and let \( \mu^x, V^x, G^x, Z^x \) denote the various quantities for an m-mode
quantum Gaussian state $\sigma$. Then the relative entropy $D(\rho\|\sigma)$ is given by the following formula:

$$D(\rho\|\sigma) = \frac{1}{2\ln2} \left[ \ln \left( \frac{Z_\sigma}{Z_\rho} \right) + \frac{1}{2} \text{Tr}[\rho^T \Delta] + \delta^T G^\sigma \delta \right].$$

(H11)

The formula in (H11) was established by [Che05] for the zero-mean case, by [Kru06] for the case of non-zero mean but equal covariance matrices, and then extended by [Pir17] to the case of general multi-mode Gaussian states. The relative entropy variance is given by the following formula [WTLB17]:

$$V(\rho\|\sigma) = \frac{1}{8\ln^22} \left[ \text{Tr}[(\Delta V)^2] + \text{Tr}[(\Delta^2)^2] \right] + \frac{1}{2\ln^22} \delta^T G^\sigma V^\sigma G^\sigma \delta,$$

(H12)

where

$$\delta := \mu^\rho - \mu^\sigma,$$

(H13)

$$\Delta := \Sigma^\sigma - \Sigma^\rho.$$

(H14)

Recall from (41) and (42) that the Holevo information and Holevo information variance of a general ensemble $\{p_Y(y), \rho^\rho_E\}_y$ are given by the following, with sums replaced by integrals:

$$I(Y; E) = \int dy \ p_Y(y) D(\rho^\rho_E\|\rho_E),$$

(H15)

$$V(Y; E) = \int dy \ p_Y(y) \left[ V(\rho^\rho_E\|\rho_E) + (D(\rho^\rho_E\|\rho_E))^2 \right] - [I(Y; E)]^2,$$

(H16)

where

$$\rho_E := \int dy \ p_Y(y) \rho^\rho_E.$$

(H17)

Then the proof of Proposition 3 is as follows:

**Proof of Proposition 3.** Recall Definition 2 for a Gaussian ensemble of quantum Gaussian states. First, consider that the expected density operator $\rho_E$ in (H17) is a quantum Gaussian state because it is a Gaussian mixture of Gaussian states. Furthermore, the entries $\mu_E^k$ of the mean vector $\mu_E$ of $\rho_E$ are given by

$$\mu_E^k := \text{Tr}[\hat{r}_j \rho_E] = \int dy \ p_Y(y) \text{Tr}[\hat{r}_j \rho^\rho_E] = \int dy \ p_Y(y) \left[ \{W y\}_j + \nu_j \right] = \{W \mu + \nu\}_j,$$

(H18)

(H19)

(H20)

(H21)

so that

$$\mu_E = W \mu + \nu.$$

(H22)

The entries $V_E^{jk}$ of the covariance matrix $V_E$ of $\rho_E$ are given by

$$V_E^{jk} := \text{Tr} \left[ \{\hat{r}_j - \mu_E^j, \hat{r}_k - \mu_E^k\} \rho_E \right] = \text{Tr} \left[ \{\hat{r}_j, \hat{r}_k\} \rho_E \right] - 2 \mu_E^j \mu_E^k \text{Tr}[\hat{r}_k \rho_E]$$

$$- 2 \mu_E^k \mu_E^j \text{Tr}[\hat{r}_j \rho_E] + 2 \mu_E^k \mu_E^j \text{Tr}[\rho_E] = \text{Tr} \left[ \{\hat{r}_j, \hat{r}_k\} \rho_E \right] - 2 \mu_E^j \mu_E^k.$$ (H23)

(H24)

(H25)

Let us focus on the first term $\text{Tr} \left[ \{\hat{r}_j, \hat{r}_k\} \rho_E \right]$. Set $y_c := y - \mu$, and consider that

$$\text{Tr} \left[ \{\hat{r}_j, \hat{r}_k\} \rho_E \right] = \int dy \ p_Y(y) \text{Tr} \left[ \{\hat{r}_j, \hat{r}_k\} \rho^\rho_E \right]$$

$$= \int dy \ p_Y(y) \left( V^{jk} + 2 [W y + \nu]_j [W y + \nu]_k \right)$$

$$= V^{jk} + 2 \int dy \ p_Y(y) [W y_c + \mu_E]_j [W y_c + \mu_E]_k,$$

(H26)

(H27)

(H28)

(H29)

(H30)

where the second equality follows from the definition of the quantum covariance matrix $V$ of $\rho^\rho_E$ and the fact that $W y + \nu$ is the mean vector of $\rho^\rho_E$. The last equality follows from (H22) and (H26). Focusing on the second term, we find that

$$\int dy \ p_Y(y) [W y_c + \mu_E]_j [W y_c + \mu_E]_k$$

$$\begin{aligned}
&= \int dy \ p_Y(y) \left( \mu_E^j + \sum_{\ell} W_{j\ell} y_c^\ell \right) \left( \mu_E^k + \sum_{m} W_{k\ell} y_c^m \right) \\
&= \mu_E^j \mu_E^k + \sum_{\ell, m} W_{j\ell} W_{k\ell} \int dy \ p_Y(y) y_c^\ell y_c^m \\
&= \mu_E^j \mu_E^k + \sum_{\ell, m} W_{j\ell} W_{k\ell} \Sigma_{\ell m} \\
&= \mu_E^j \mu_E^k + \left[ W \Sigma W^T \right]_{jk},
\end{aligned}$$

(H31)

(H32)

(H33)

(H34)

where the second equality follows because

$$\int dy \ p_Y(y) \sum_{\ell} W_{j\ell} y_c^\ell \mu_E^k = 0,$$

(H35)

with similar reasoning for the other vanishing term. It follows that

$$\text{Tr} \left[ \{\hat{r}_j, \hat{r}_k\} \rho_E \right] = V^{jk} + 2 \left[ \mu_E^j \mu_E^k + W \Sigma W^T \right]_{jk},$$

(H36)

and we find from combining with (H25) that

$$V_E^{jk} = V^{jk} + 2 \left[ W \Sigma W^T \right]_{jk}.$$
or equivalently,
\[ V_E = V + 2W\Sigma W^T. \] (H38)
So the expected density operator \( \rho_E \) is a quantum Gaussian state with mean vector given by (H22) and quantum covariance matrix given by (H38). The normalization \( Z_E \) of \( \rho_E \) is thus given by
\[ Z_E := \det([V_E + i\Omega]/2), \] (H39)
and the Hamiltonian matrix \( G_E \) of \( \rho_E \) is given by
\[ G_E := 2\Omega \arcoth(iV_E\Omega). \] (H40)
Thus, the Holevo information \( I(Y; E) \) works out to
\[ I(Y; E) = \int dy \ p_Y(y) D(\rho^y_E | \rho_E) \] (H41)
\[ = \int dy \frac{p_Y(y)}{2\ln 2} \left[ \ln \left( \frac{Z_E}{Z} \right) + \frac{1}{2} \Tr[V\Delta] + \delta^T G_E \delta \right] \] (H42)
\[ = \frac{1}{2\ln 2} \left[ \ln \left( \frac{Z_E}{Z} \right) + \frac{1}{2} \Tr[V\Delta] + \int dy \ p_Y(y) \delta^T G_E \delta \right], \] (H43)
where
\[ \delta := Wy + \nu - (W\mu + \nu) = W(y - \mu). \] (H44)
For the equality in (H43), we applied the formula in (H11). To evaluate the last integral, consider that
\[ \int dy \ p_Y(y) \delta^T G_E \delta \]
\[ = \int dy \ p_Y(y) \Tr[\delta \delta^T G_E] \] (H45)
\[ = \int dy \ p_Y(y) \Tr[W(y - \mu)(y - \mu)^T W^T G_E] \] (H46)
\[ = \Tr[W\Sigma W^T G_E]. \] (H47)
Then the formula for the Holevo information \( I(Y; E) \) reduces to
\[ I(Y; E) = \frac{1}{2\ln 2} \left[ \ln \left( \frac{Z_E}{Z} \right) + \frac{1}{2} \Tr[V\Delta] + \Tr[W\Sigma W^T G_E] \right], \] (H48)
as claimed.

We now determine a formula for the Holevo information variance. We first consider the difference
\[ \int dy \ p_Y(y) (D(\rho^y_E | \rho_E))^2 - [I(Y; E)]^2. \] (H49)
Consider from (H43) that
\[ (2\ln 2)^2 \left[ (D(\rho^y_E | \rho_E))^2 - [I(Y; E)]^2 \right] \]
\[ = \left[ \ln \left( \frac{Z_E}{Z} \right) + \frac{1}{2} \Tr[V\Delta] + \delta^T G_E \delta \right]^2 \]
\[ - \left[ \ln \left( \frac{Z_E}{Z} \right) + \frac{1}{2} \Tr[V\Delta] + \Tr[W\Sigma W^T G_E] \right]^2 \] (H50)
\[ = 2 \left( \ln \left( \frac{Z_E}{Z} \right) + \frac{1}{2} \Tr[V\Delta] \right) (\delta^T G_E \delta - \Tr[W\Sigma W^T G_E]) \]
\[ + (\delta^T G_E \delta)^2 - (\Tr[W\Sigma W^T G_E])^2. \] (H51)
This means that
\[ (2\ln 2)^2 \int dy \ p_Y(y) (D(\rho^y_E | \rho_E))^2 - [I(Y; E)]^2 \]
\[ = \int dy \ p_Y(y) (\delta^T G_E \delta)^2 - (\Tr[W\Sigma W^T G_E])^2, \] (H52)
due to (H48). To evaluate the first term, consider that
\[ \int dy \ p_Y(y) (\delta^T G_E \delta)^2 \]
\[ = \int dy \ p_Y(y) (y_c^T W^T G_E W y_c)^2. \] (H53)
Then write the above as
\[ \int dy \ p_Y(y) \sum_{ijkl} y_c^i W^T G_E W y_c^j y_c^k W^T G_E W y_c^l \]
\[ = \sum_{ijkl} [W^T G_E W]_{ij} [W^T G_E W]_{kl} \int dy \ p_Y(y) y_c^i y_c^j y_c^k y_c^l \] (H54)
\[ = \sum_{ijkl} [W^T G_E W]_{ij} [W^T G_E W]_{kl} \times \]
\[ \left[ \Sigma^{ij} \Sigma^{kl} + \Sigma^{ik} \Sigma^{jl} + \Sigma^{il} \Sigma^{jk} \right] \] (H55)
\[ = (\Tr[W^T G_E W \Sigma])^2 + 2 \Tr[(W^T G_E W \Sigma)^2] \] (H56)
\[ = (\Tr[W\Sigma W^T G_E])^2 + 2 \Tr[(W\Sigma W^T G_E)^2], \] (H57)
where we applied Isserlis’ theorem [Issi18] to evaluate the fourth moment and we employed the facts that \( W^T G_E W \) and \( \Sigma \) are symmetric matrices. So then by combining with (H53), we find that
\[ \int dy \ p_Y(y) (D(\rho^y_E | \rho_E))^2 - [I(Y; E)]^2 \]
\[ = \frac{1}{2\ln^2 2} \Tr[(W\Sigma W^T G_E)^2]. \] (H58)
It remains to evaluate the term
\[ \int dy \ p_Y(y) V(\rho^y_E | \rho_E) \]
\[ = \int dy \frac{p_Y(y)}{8\ln^2 2} \left[ \Tr[(\Delta V)^2] + \Tr[(\Delta \Omega)^2] + 4\delta^T G_E V G_E \delta \right]. \] (H59)
where we applied the formula in (H12). Then it follows that
\[
\begin{align*}
&\int dy \rho_Y(y) \delta^T G_E V G_E \delta, \\
&= \int dy \rho_Y(y) \text{Tr}[\delta^T G_E V G_E] \\
&= \int dy \rho_Y(y) \text{Tr}[W (y - \mu) (y - \mu)^T W^T G_E V G_E] \\
&= \text{Tr}[W \Sigma W^T G_E V G_E].
\end{align*}
\]
Putting everything together, we find that
\[
V(Y; E) = \frac{1}{8 \ln^2 2} \left[ \text{Tr}[(\Delta V)^2] + \text{Tr}[(\Delta \Omega)^2] \right] \\
+ \frac{1}{2 \ln^2 2} \left[ \text{Tr}[W \Sigma W^T G_E V G_E] + \text{Tr}[(W \Sigma W^T G_E)^2] \right],
\]
as claimed. ■

The formulas from Proposition 3 can be applied to the scenario in which some modes of a Gaussian state are measured according to a “general-dyne” Gaussian measurement [GLS16, Ser17], which leaves a Gaussian ensemble of Gaussian states on the remaining modes. To see how this works, let \( \rho_{AB} \) denote a bipartite Gaussian state of \( m + n \) modes, with \( m \) modes for system \( A \) and \( n \) modes for system \( B \). Suppose that the \( (m + n) \times 1 \) mean vector of \( \rho_{AB} \) is
\[
\begin{pmatrix}
\bar{\tau}_A \\
\bar{\tau}_B
\end{pmatrix},
\]
and the \( (m + n) \times 2 (m + n) \) quantum covariance matrix is
\[
\begin{pmatrix}
V_A & V_{AB} \\
V_{AB}^T & V_B
\end{pmatrix}.
\]
A general-dyne measurement of system \( B \) is described by a quantum Gaussian state \( \omega_M \) with covariance matrix \( V_M \) satisfying the uncertainty principle \( V_M + i \Omega \geq 0 \) [GLS16, Ser17]. The POVM elements of this general-dyne detection are given by
\[
\left\{ \frac{1}{(2\pi)^{m+n}} \hat{D}_{-y} \omega_M \hat{D}_y \right\}_{y \in \mathbb{R}^{2n}},
\]
where the displacement operator is defined as \( \hat{D}_y := \exp(iy^T \Omega r) \), and the following completeness relation holds
\[
\frac{1}{(2\pi)^m} \int_{\mathbb{R}^{2n}} dy \hat{D}_{-y} \omega_M \hat{D}_y.
\]