Bell nonlocality threshold in device-independent quantum key distribution

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We define, for any bipartite Bell scenario, a device-independent key rate that is a proper measure of nonlocality, assuming each party randomly picks at each round one of the available measurements to generate its raw key. A positive value of it ensures that a secret key can be established. Any continuous nonlocality measure $N$ sets a nonnegative lower bound on it that is nondecreasing with $N$. There can thus be a threshold for the amount of nonlocality, as quantified by $N$, above which a secret key is surely achievable. We find such a threshold for two two-outcome measurements per party.

I. INTRODUCTION

Using a secret sequence of characters, termed a key, for encryption and decryption, allows to transmit a message in an absolutely confidential way. The aim of quantum key distribution (QKD) studies is to examine whether two distant legitimate users, usually named Alice and Bob, can establish such a key in the presence of an eavesdropper, Eve, within the framework of quantum mechanics [1]. To do so, Alice and Bob need at least to be able to process and exchange classical information and each to choose one out of several measurements to perform on quantum systems. The communication channel between them is public. Namely, any message sent over it becomes known to all parties. Moreover, Alice’s and Bob’s quantum systems in general share a global state with systems that Eve can manipulate as she wishes. On the other hand, Eve does not know which measurements Alice and Bob actually perform, the outcomes they get and the results of their classical computations. The first security analyses of QKD schemes apply only to specific quantum systems Hilbert spaces and measurement operators on these spaces [12]. Consequently, a concrete implementation must follow the ideal model exactly.

Device-independent QKD (DIQKD) protocols, on the contrary, do not require that Alice and Bob know anything about the sizes and states of the quantum systems and about the measurement devices [8–9]. They can only estimate the probabilities of the measurement outcomes. To establish a common and secret key, they first generate raw keys using measurement outcomes. These keys are not fully confidential and not completely identical to each other. Alice and Bob change them into the final key with the help of the above mentioned classical means. In Refs. [8–9], only the so-called collective attacks, during the generation of the raw key, are considered. Namely, it is assumed that Eve prepares a tripartite quantum system in the same state several times and that Alice’s and Bob’s possible measurements are the same each time. But the measurements may actually be performed on a global system which is not necessarily in a product state and the measurement devices may work differently from one round to another [10–11]. Furthermore, these apparatuses may have internal memories [12–13]. The security of a DIQKD protocol against these most general attacks follows from that against collective attacks [13].

Device-dependent QKD is closely related to quantum entanglement. Some proposed protocols rely on entangled Alice’s and Bob’s quantum systems [3, 5]. Moreover, the security of those known as prepare-and-measure protocols, for which such quantum correlations are absent, results from that of corresponding entanglement-based protocols [4, 6, 7]. Entanglement is a useful resource for many tasks and different measures of the entanglement of quantum states, appropriate for different tasks, have been introduced [14]. A proper measure, called an entanglement monotone, vanishes for separable states [15] and is nonincreasing under local operations and classical communication, since a quantum state cannot be changed into a more entangled one using only these means [14–16, 19]. The distillable key rate, defined for a given legitimate QKD users’ state, satisfies these requirements [14, 20, 21]. In DIQKD, since Alice and Bob can only estimate joint probability distributions, the relevant resource is not entanglement but more likely Bell nonlocality [8, 9, 22–23], whose relation to entanglement is not straightforward [15, 24, 26].

In this paper, we are interested in Bell nonlocality as a resource for DIQKD and in its quantification. We first introduce, for any numbers of choosable measurements and measurement outcomes, a device-independent key rate $R$. It is defined, under the assumption of collective attacks, by considering a class of protocols, to generate the raw keys, which involve processing and publicly exchanging classical information and randomly choosing at each round, for each legitimate user, one among all the possible measurements. The usual protocols that consist in using only two preselected measurements belong to this class. A confidential key can surely be established when $R$ is positive but not when it is zero. The rate $R$ is a proper measure of nonlocality, i.e., it vanishes for Bell local sets of probabilities and is nonincreasing under the relevant operations [27]. We name such measures as nonlocality monotones. We show that any continuous nonlocality monotone $N$ sets a tight lower bound on $R$ that is nondecreasing with $N$ and vanishes when $N$ does. Thus, either this bound is trivial and nothing can be inferred from $N$ alone about the achievability of a secret key, or there is a threshold value for the amount of nonlocality, as quantified by $N$, above which Alice and Bob
are certain that such a key can be established, without needing to evaluate any other quantity.

II. ALICE AND BOB’S POSSIBLE OPERATIONS

The following situation is considered throughout the paper. Alice and Eve initially share a quantum system in the state $\rho$. Alice (Bob) can choose one of $m \,(n)$ measurements to perform on her (his) subsystem with Hilbert space $\mathcal{H}_A \,(\mathcal{H}_B)$. The legitimate users know nothing about the quantum system, its state and the measurement devices. In more precise terms, Alice (Bob) can observe one of $m \,(n)$ classical random variables $A_x \,(B_y)$. Alice and Bob can only get information on the probability mass functions $P_{A_x,B_y}$ denoted $P_{x,y}$ in the following. The indices $x$ and $y$ are usually termed as inputs and the outcomes of the random variables $A_x \,$ and $B_y$ as outputs. Without loss of generality, it can be assumed that all variables $A_x \,$ ($B_y$) have the same set $\mathcal{A} \,(\mathcal{B})$ of outputs by adding zero probability outcomes. These sets are referred to as alphabets. Obviously, $m \,, n \,, \mathcal{A}$ and $\mathcal{B}$ are known to Alice and Bob. The random variable $A_x \,$ ($B_y$) corresponds to a set of positive operators $M_{x,a} \,$ ($N_{y,b}$) such that $\sum_{a \in \mathcal{A}} M_{x,a} \left( \sum_{b \in \mathcal{B}} N_{y,b} \right)$ is the identity operator on $\mathcal{H}_A \,(\mathcal{H}_B)$ and

$$P_{x,y}(a,b) = \text{tr}(\rho M_{x,a} \otimes N_{y,b} \otimes I_E),$$

where $I_E$ is the identity operator on Eve’s Hilbert space $\mathcal{H}_E$. A distribution tuple $\mathbf{P} = (P_{x,y}(a,b))_{x,y,a,b}$ is said to be quantum if it can be written in this form with appropriate state and measurement operators.

In addition to the $A_x \,$ and $B_y$, Alice and Bob can create random variables uncorrelated to the $A_x \,$ and $B_y$ and available at first only to one of them. Each can also compute new random variables from preexisting ones and use a classical communication channel. Any message sent over this channel becomes known to the three parties and it is the only way to get a random variable from another party. It is not necessary to introduce explicitly additional variables for Eve since they can be taken into account by considering suitable system, state $\rho$ and measurements on her subsystem. Let us be more specific about how the $A_x$, that cannot be observed simultaneously, are employed. At some stage, Alice uses one of the random variables at her disposal, say $X$, with alphabet in $\{1, \ldots, m\}$, to choose which $A_x$ to observe. More precisely, she generates $U$ according to $U = A_x$ when $X = x$. Bob uses the $B_y$ and $Y$ with alphabet in $\{1, \ldots, n\}$ in a similar way to produce the random variable $V$, see Fig1.

III. RAW KEY PROTOCOLS

To generate their raw keys, using the $A_x$ and $B_y$, Alice and Bob proceed as follows. First, they create some random variables and send some of them over the public channel. Then, they calculate new ones and subsequently produce the $U$ and $V$ as explained above. Finally, they generate $A$ and $B$ from all the available random variables. Alice’s (Bob’s) raw key is a sequence of independent realizations of $A \,(B)$. All the just mentioned classical random variables but $U$, $V$, $A$ and $B$ are quantum-mechanically described by the state

$$\hat{\rho} = \sum_{x,y,a} P_{X,Y,E}(x,y,a)\Pi_{A_x}^{Alice} \otimes \Pi_{B_y}^{Bob} \otimes \Pi_{E}^{Eve},$$

where $E$ is a tuple made up of the public ones and $X \,(Y)$ is a component of $X \,(Y)$ or of $E$. From their definitions, $X$ and $Y$ are conditionally independent given $E$, i.e., $P_{X,Y,E} = P_{X|E} P_{Y|E} P_{E}$. The $\Pi_{A_x}^{Alice} \,(\Pi_{B_y}^{Bob}, \Pi_{E}^{Eve})$ are rank-one projectors whose sum is the identity operator on a Hilbert space $\mathcal{H}_A \,(\mathcal{H}_B, \mathcal{H}_E)$. At the end of the raw key protocol, the three parties share the state

$$\rho_{rk} = \sum_{a,b} \Pi_a \otimes \Pi_b \otimes \text{tr}_{\mathcal{H}_{AB}} (\hat{\rho} M_a \otimes N_b \otimes I_E'),$$

where $\rho' = \hat{\rho} \otimes \rho' , I_E'$ is the identity operator on $\mathcal{H}_E \otimes \mathcal{H}_E$, $\Pi_a \,(\Pi_b)$ denotes mutually orthogonal rank-one projectors and $\text{tr}_{\mathcal{H}_{AB}}$ the partial trace over the Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_E$, see Appendix A. Observing $A$ and $B$ means performing the measurement with operators $\Pi_a \otimes \Pi_b \otimes I_E'$ on $\rho_{rk}$. The positive operator $M_a$ reads

$$M_a = \sum_{x,e,u} P_{A|U,X,E}(a|u,x,e)\Pi_{x,e}^{Alice} \otimes M_{x,u},$$

where $x$ corresponds to $X$ and the conditional probability mass function $P_{A|U,X,E}$ is determined by the protocol. The operators $N_b$ are given by similar expressions.
Equation 3 shows that the correlations between Alice, Bob and Eve at the end of the raw key protocol are formally identical to those obtained by performing the measurement with operators $M_x \otimes N_y \otimes I_L'$ on $\rho'$. The simple protocol in which Alice and Bob each choose a particular input, say $\xi$ and $\zeta$, is obviously one of those considered here. In this case, there is no public random variables, $P_X(x) = \delta_{x,\xi}$, $P_Y(y) = \delta_{y,\zeta}$, $A = U$ and $B = V$ and so the last term of eq.(3) simplifies to $\text{tr}_{H_A \otimes H_B}(p M_{x,a} \otimes N_{y,b} \otimes I_L')$. Strictly speaking, the above is only valid when Eve merely collects the public information in the course of the raw key protocol. However, any Eve’s measurement during which it can equivalently be taken into account as a measurement on $\rho_{rk}$, see Appendix A. Thus, it can be considered as being performed amid the protocol generating the private key.

IV. DEVICE-INDEPENDENT KEY RATE

Let $\omega$ be a state of the form of eq.(3), $l(\omega)$ the length of the longest secret key that Alice and Bob can achieve when they share $\omega^{\otimes L}$ with Eve and $R'(\omega)$ the large $L$ limit of $l(\omega)/L$ [21, 28]. We define, for any quantum distribution tuple $\rho$, the device-independent key rate

$$R(\rho) = \inf_{\rho, (M_{x,a})_a, (N_{y,b})_b} \sup_{r_{rk}} R'(\rho_{rk}),$$

(5)

where the supremum is taken over all the raw key protocols described above, the infimum is taken over all the $\rho$, $(M_{x,a})_a$ and $(N_{y,b})_b$ satisfying eq.(1) with $\rho$ and $\rho_{rk}$ is given by eqs.(1)-5 with the probability mass functions of the protocol $r_{rk}$. The rate $R$ is nonnegative by construction. Whenever Alice’s and Bob’s random variables are described by the distributions $P_{x,y}$, they can establish, in the limit of large $L$, a secret key of length at least equal to $LR(\rho)$ from raw keys of $L$ characters generated using an appropriate raw key protocol. In particular, a privy key can surely be generated as soon as $R(\rho) > 0$. If $R(\rho) = 0$, there are states and measurement operators fulfilling eq.(1) with $\rho$ for which a confidential key cannot be achieved.

As we will see, $R$ preserves the Bell nonlocality order defined as follows. Consider two distribution tuples $\rho$ and $\rho'$ consisting of non-signaling probabilities with the same output alphabets and numbers of inputs. The former is not less nonlocal than the latter if the probabilities $P_{x,y}(a,b)$ can be obtained from the $P_{x,y}(a,b)$ by performing operations which are compositions of input and output relabelings, output coarse grainings and input substitutions and by mixing the results of such operations and with any Bell local distribution tuple [27]. For quantum $\rho$ and $\rho'$ related in this way, one has $R(\rho') \leq R(\rho)$. This monotonicity of $R$ can be proved using the Lemma below. We remark that the nonlocality order is partial, i.e., for some pairs of distribution tuples, none of the two can be transformed into the other by the operations just mentioned.

Lemma. Let $\rho$ and $\rho'$ be two distribution tuples with output alphabets $A$ and $B$ and numbers $m$ and $n$ of inputs such that $\rho$ is not less nonlocal than $\rho'$ and $A_x$ and $B_y$ be random variables such that $P_{A_x,B_y} = P_{x,y}$.

There are a random integer $K$ and tuples $\tilde{A}, \tilde{B}$ of the form $P_{K,P_{A},\tilde{B}}$, where $A_x$ and $B_y$ have alphabets $A$ and $B$, respectively, self-maps $F_{x,k}$ and $G_{y,k}$ and inputs $z(x,k)$ and $t(y,k)$ such that the distributions of

$$(A'_x, B'_y) = (\tilde{A}_x, \tilde{B}_y)$$

if $K = 0$

$$= (F_{x,k}(A_{x}(x,k)), G_{y,k}(B_{t(y,k)}))$$

if $K = k \geq 1,$

(6)

are given by $P_{A'_x,B'_y} = P'_{x,y}$.

If $\rho$ is quantum then also is $\rho'$.

The proofs of the Lemma and Propositions are given in Appendices B, C and D. This Lemma ensures that, from given $A_x$ and $B_y$ with distributions $F_{x,y}$, Alice and Bob have effectively access to random variables characterized by any distribution tuple $\rho'$ not more nonlocal than $\rho$, by proceeding as follows. Alice creates the corresponding $K$, $\tilde{A}_x$ and $\tilde{B}_y$ and sends $K$ and the $\tilde{B}_y$ to Bob. Then, she generates, in sequence, the random variables $X'$, $Y$ which are $X'$ if $K = 0$ and $z(X',k)$ if $K = k \geq 1$, $U$ according to $U = A_x$ when $X = x$ and, finally, $U'$ which is $\tilde{A}_x$ if $(K, X') = (0, x')$ and $F_{z,k}(U)$ if $(K, X') = (k, x')$ with $k \geq 1$. Bob does similar operations using $K$, the $\tilde{B}_y$ and $U'$, see Fig.1. In this Figure, it is assumed, to simplify, that $K \geq 1$. The above produces the same $U'$ and $V'$ as $U' = A'_x$, when $X' = x'$ and $V' = B'_y$ when $Y' = y'$ where $A'_x$ and $B'_y$ are given by eq.(6). Note that Eve gets $K$ and the $\tilde{B}_y$ which are sent over the public channel.

Using the above Lemma, the following can be shown.

Proposition 1. The function $R$ given by eq.(5) has the properties:

(i) $R$ preserves the nonlocality order.

(ii) $R$ vanishes for Bell local distribution tuples.

A function fulfilling these two requirements is a nonlocality monotone, i.e., a proper measure of Bell nonlocality [27]. The above Proposition implies that the device-independent key rate (5) is a nonlocality monotone. Property (ii) can be seen as a consequence of the fact that a secret key cannot always be established and of (i) as follows. Any distribution tuple is not less nonlocal than any Bell local one. Thus, due to property (i), $R$ assumes its minimum value for Bell local distribution tuples. If this minimum were nonzero then a secret key could be produced in any case. Proposition shows that a private key can surely be generated for any distribution tuple not less nonlocal than a given one for which this is possible. Besides, a confidential key can be established with certainty only for nonlocal distribution tuples. Proposition does not ensure that the converse
holds. There may be nonlocal distribution tuples \( P \) such that a privy key cannot be achieved for some states and measurement operators fulfilling eq. (1) with \( P \).

V. CONTINUOUS NONLOCALITY MONOTONES

According to the above Proposition and definition, the device-independent key rate \( R \) quantifies both the efficiency in secret key generation and the amount of Bell nonlocality of a distribution tuple. However, it is not straightforward to evaluate. Moreover, one may prefer a measure that vanishes only for Bell local distribution tuples. It is then of interest to consider other nonlocality monotones. For that purpose, we use the following result.

**Proposition 2.** Let \( Q \) and \( L \) be the sets of quantum and Bell local distribution tuples, respectively.

For any nonlocality monotone \( M \) on \( Q \) and nonnegative continuous function \( N \) on \( Q \) which vanishes on \( L \), there is a nondecreasing function \( f \) on \( I = [0, N_m] \), where \( N_m \) is the maximum value of \( N \) on \( Q \), such that \( f(0) = 0 \), \( f \circ N \leq M \), and, for any \( s \in I \) and \( \epsilon > 0 \), there is \( P \in Q \) for which \( N(P) = s \) and \( M(P) < f(s) + \epsilon \).

Whenever Alice’s and Bob’s random variables are described by the distributions \( P_{x,y} \), they can generate a secret key with a rate no lower than \( f \circ N(P) \) where \( N \) is any continuous nonlocality monotone and \( f \) is given by the above Proposition with \( N \) and \( M = R \). This remains valid if \( f \) is replaced by other nondecreasing functions but \( f \) is the greatest one. If \( f \circ N(P) = 0 \), there exists, for any \( \epsilon > 0 \), a quantum distribution tuple \( P' \) such that \( N(P') = N(P) \) and \( R(P') < \epsilon \). So, in this case, nothing can be inferred from the value \( N(P) \) regarding the possibility of establishing a confidential key. On the contrary, \( f \circ N(P) > 0 \) ensures that a private key can be generated. This condition can be rewritten as \( N(P) > N^* \) where \( N^* = \sup \{ s \in I : f(s) = 0 \} \) is set only by the measure \( N \). By definition, \( N^* \) is not larger than the maximum value \( N_m \). If \( N^* = N_m \), \( f \circ N = 0 \) and it cannot be determined whether a secret key can be established by evaluating only \( N \). By contrast, for a measure \( N \) such that \( N^* < N_m \), \( N^* \) is a threshold value above which a privy key can be achieved with certainty. Proposition 2 does not require that \( N \) is a nonlocality monotone but only that it is continuous and vanishes for Bell local tuples. For instance, \( N \) can be defined from a Bell inequality. Proposition 2 applies to such measures though they are not nonlocality monotones in general.

We now consider the particular case of numbers of inputs \( m = n = 2 \) and alphabets \( A \) and \( B \) consisting of two outputs, that cannot be assumed to be -1 and 1, for which the Clauser-Horne-Shimony-Holt inequality violation

\[
\hat{N}(P) = \max \left\{ 0, \max_{\nu} \left| \sum_{x,y=1}^{2} \nu(x,y) \langle A_x B_y \rangle - 2 \right| \right\}, \quad (7)
\]

is a nonlocality monotone, as shown below. In this expression, the maximum is taken over all the maps \( \nu : \{1,2\}^2 \to \{-1,1\} \) assuming the value -1 only once and (C) denotes the expectation of the random variable \( C \). The measure (7) vanishes for Bell local distribution tuples and only for them. To see that it preserves the nonlocality order, first note that it is a convex function of its argument. Moreover, the right side of eq. (7) is not modified by an input relabeling. An output relabeling is equivalent to changing the sign of one of the random variables in eq. (7), and so also does not alter the value of \( \hat{N} \). An input substitution is the same as setting \( A_1 = A_2 \) or \( B_1 = B_2 \) in eq. (7) which gives \( \hat{N} = 0 \). An output coarse graining is equivalent to replacing one of the random variables in eq. (7) by 1 which also leads to \( \hat{N} = 0 \). As is well known, the set of the possible values of \( \hat{N} \) is the interval \([0,2(\sqrt{2} - 1)]\). A nondecreasing function \( g \) such that \( R \geq g \circ \hat{N} \) can be found, see Appendix E. It results from its expression that there is a threshold value \( \hat{N}^* \leq 0.652 < 2(\sqrt{2} - 1) \) for the nonlocality monotone (7) above which a private key can surely be generated. The existence of \( \hat{N}^* \) can be seen as follows. For any \( P \) such that \( \hat{N}(P) > 0 \), there are inputs \( \xi \) and \( \zeta \) for which \( \langle AB \rangle = \langle A_{\xi} B_{\zeta} \rangle \) is finite. Consider a raw key protocol generating \( A = ZA_{\xi} \) and \( B = ZB_{\zeta} \) where \( Z \) is a public equally distributed random variable with alphabet \([-1,1]\). The resulting rate \( R'(\rho_{AB}) \) in eq. 5, and hence \( R(P) \), is not lower than \( I(\langle AB \rangle) - r \circ \hat{N} \) where \( I \) is the mutual information between \( A \) and \( B \) that depends only on \( \langle AB \rangle = \langle A_{\xi} B_{\zeta} \rangle \) and \( r \) is a continuous nonincreasing function with \( r(2\sqrt{2} - 2) = 0 \). The function \( g \) can be obtained by noting that there are \( \xi \) and \( \zeta \) such that \( |\langle AB \rangle| \geq 1/2 + \hat{N}(P)/4 \). Other raw key protocols are used in Appendix E.

VI. SUMMARY AND OPEN QUESTIONS

In summary, a device-independent key rate has been introduced and shown to be a nonlocality monotone. Moreover, it has been proved that there are only two possibilities for any continuous nonlocality monotone. Either it can never be decided whether a secret key can be established by evaluating only this measure, or there is a threshold value for it above which this is surely achievable. A readily computable nonlocality monotone with such a threshold has been found for two two-outcome measurements per legitimate user. The defined device-independent key rate may vanish for some nonlocal sets of probabilities. Were this not to be the case, Bell nonlocality would be a necessary and sufficient condition for DIQKD with raw key protocols. This may be correct only for some numbers of choosable measurements and measurement outcomes. Related to this issue, it would be interesting to improve the upper bound on the threshold value of the aforementioned particular nonlocality monotone. Since this measure vanishes only for Bell local sets...
of probabilities, a threshold value of zero would prove the above mentioned equivalence in this case. The answers to these open questions may depend on the considered class of raw key protocols. It can be further enlarged, for instance, by dropping the assumption made here that no information is exchanged after the measurements.

Appendix A: Derivation of equation (3)

To simplify, the random variables transmitted over the public channel at the same stage of the raw key protocol are here grouped into one. After receiving the value $e_1$ of the first one $E_1$, Eve performs a measurement on her subsystem. This generates a random variable $E'_1$ and $\rho$ is changed into $\Lambda_{1,e'_1}(\rho)/p_{e_1,e'_1}$ when $E'_1 = e'_1$ when $p_{e_1,e'_1} = \text{tr}\Lambda_{e_1,e'_1}(\rho)$. The Kraus operators of the quantum operation $\Lambda_{e_1,e'_1}$ are of the form $I_A \otimes I_B \otimes K_{e_1,e'_1,i}$ where $I_A$ ($I_B$) is the identity operator on $\mathcal{H}_A$ ($\mathcal{H}_B$). The probabilities $p_{e_1,e'_1}$ satisfy $\sum_{e'_1} p_{e_1,e'_1} = 1$. A deterministic operation, e.g., the identity operation, is a measurement with a single outcome $e'_1$. Moreover, sequential measurements can be considered as a single one with a properly defined $E'_1$. The set of the values $e'_1$ may depend on $e_1$. However, it can be assumed, without loss of generality, that it does not, by adding zero probability outcomes, and hence that there is a unique $E'_1$ with $P_{E'_1|E_1}(e'_1|e_1) = p_{e_1,e'_1}$. Repeating these arguments for all components of $E$ leads to the random tuple $E'_1$, conditional distribution $P_{E'_1|E}$ and quantum operations $\Lambda_{e,e'_1}$ with Kraus operators $I_A \otimes I_B \otimes K_{e,e'_1,i}$.

The probability mass function of $X, Y, E, E', U$ and $V$ is $P_{X,Y,E|E'}P_{E'|E}P_{U,V|X,Y,E,E'}$ where the last conditional distribution is given by

$$P(u,v|x,y,e,e') = \text{tr}(\Lambda_{e,e'}(\rho)M_{x,u}N_{y,v}I_{E'})/P(e'|e),$$

with the appropriate identity operator $I_{E'}$ and omitting the subscripts for the distributions. For given values of these random variables, Eve’s state is proportional to $\rho_{e,e'} = \text{tr}(\Lambda_{e,e'}(\rho)M_{x,u}N_{y,v}I_{E'})$ where $\rho_{e,e'}$ is the quantum operation with Kraus operators $K_{e,e',i}$. The marginal distribution $P_{A,B,E,E'}$ directly follows with the conditional distributions $P_{A|U,X,E}$ and $P_{B|U,Y,E}$ of the protocol. Using $P_{X,Y,U,V|A,B,E,E'}$, one finds that Eve’s state for $A = a, B = b, E = e$ and $E' = e'$ is

$$\omega_{a,b,e,e'} = \Lambda_e \left( \Pi_{e}^{E_{1e}} \otimes \sum_{x,y,u,v} P(a|u,x,e)P(b|v,y,e) \times P(x,y,e)\text{tr}_{A\otimes H_B}(\rho M_{x,u}N_{y,v}I_{E'}) \right)/P(a,b,e,e'),$$

where $\Pi_{e}^{E_{1e}} = |e\rangle\langle e|$ and $\Lambda_e$ is the quantum operation with Kraus operators $|e\rangle \otimes K_{e,e',i}$. Performing the measurement with operators $\Pi_u \otimes \Pi_b \otimes \Pi_{e}^{E_{1e}} \otimes I_{E}$ and then that characterized by the $\Lambda_e$ on the state given by eq.(3) in the main text leads to the same distribution $P_{A,B,E,E'}$ and Eve’s states $\omega_{a,b,e,e'}$.

Appendix B: Proof of the Lemma

The tuples $P$ and $P'$ are related by

$$P' = p_0L + \sum_{k \geq 1} p_k T_k(P),$$

(B1)

where the probabilities $p_k$ obey $\sum_{k \geq 0} p_k = 1$, $L$ is a Bell local distribution tuple, and $T_k$ are compositions of input and output relabellings, output coarse grainings and input substitutions [27]. The tuple $L$ can be written as $L = \sum_{a,b} q_{a,b} D_{a,b}$ where the sum runs over all the $a = (a_x)_x \in A^n$ and $b = (b_y)_y \in B^m$, the probabilities $q_{a,b}$ sum to unity and the only nonvanishing components of $D_{a,b}$, for the inputs $x$ and $y$, are those corresponding to the outputs $a = a_x$ and $b = b_y$. Consider random tuples $\tilde{A} = (A_x)_x = 1$ and $\tilde{B} = (B_y)_y = 1$ where $\tilde{A}$ and $\tilde{B}$ have alphabets $A$ and $B$, respectively, such that $P_{\tilde{A},\tilde{B}}(a,b) = q_{a,b}$. The components of $L$ are equal to the marginal probabilities $P_{\tilde{A},\tilde{B}}(a,b)$.

Let $\hat{P}$ be any distribution tuple. An input substitution acts on it as follows. The components $P_{x,y}(a,b)$ are replaced by the $P_{x,y}(a,b)$ for some given $x$ and $x'$ and the other ones remain unchanged. We denote this operation as $I(x,x')$ and similarly for given inputs $y$ and $y'$. An input relabeling consists in a permutation of the inputs $x$ or $y$ of the inputs $y$. Since any permutation can be expressed as a product of transpositions, an input relabeling can be decomposed into operations that exchange the probabilities $P_x(y,a)$ and $P_{x'}(y,a)$ for some given $x$ and $x'$ and leave the other ones unchanged, which we denote by $I(x,x'),$ and similarly for given inputs $y$ and $y'$. The input operations satisfy $I(x,y') \circ I(x,x') = I(x,x') \circ I(x,y')$ and similar commutation relations with one or both operations replaced by an input substitution.

The output operations can be decomposed into transformations that change only the probabilities $P_{xy}(a,b)$ for a given $x$ or $y$. We denote such operations as $O_x$ and $O_y$. They obey $O_x \circ O_y = O_{x'} \circ O_y$. We have also $I(x,y') \circ O_x = O_{x'} \circ I(x,y')$ for $z \neq x$ and $y', I(x,x') \circ O_y = O_{x'} \circ I(x,x') = I(x,x') \circ O_x = O_{x'} \circ I(x,x') \circ O_y = O_{x'} \circ O_y = O_{x'}$ and similar relations with the inputs $x$ and $x'$ replaced by inputs $y$ and $y'$. Consequently, any transformation $T_k$ appearing in eq.(3) can be written as $T_k = O^A_k \circ O^B_k \circ \tilde{T}_k \circ \tilde{T}_k$ where $O^A_k$ ($O^B_k$) consists of output operations for given inputs $x$ and $y$ and $\tilde{T}_k \circ \tilde{T}_k$ of operations on the inputs $x$ and $y$. Moreover, the component of $I(x,y') \circ O_x \circ \tilde{T}_k \circ \tilde{T}_k$ for the inputs $x$ and $y$ and outputs $a$ and $b$ can be expressed as $P_{x'(z,k),y(v,k)}(a,b)$ with $z(x,k)$ and $t(y,k)$ determined by $\tilde{T}_k \circ \tilde{T}_k$, respectively.

Let $\hat{P}$ be any distribution tuple with alphabets $A$ and $B$ and $C_x$ and $D_y$ random variables such that $P_{C_x,D_y} = P_{x,y}$. An output relabeling for some given $x$ acts on $\hat{P}$ as follows. The components $P_{x,y}(a,b)$ are replaced by the probabilities $P_{x,y}(\pi(a),b) = P_{x,(\pi(C_x),D_y)(a,b)}$ where $\pi$ is
a permutation on $A$ and $\pi^{-1}$ is its inverse and the other ones remain unchanged, and similarly for a given input $y$. An output coarse graining is characterized by an input, a subset of the corresponding output alphabet and an element of this subset, say $x, A'$ and $a'$, respectively. Under this operation, $\hat{P}_{x,y}(a,b)$ does not change for $a \not\in A'$, vanishes for $a \in A' \setminus \{a'\}$ and becomes $\sum_{a'' \in A'} \hat{P}_{x,y}(a'',b)$ for $a = a'$ and the other probabilities remain the same, and similarly for given $y, B' \subset B$ and $b' \in B'$. The components for $x$ of the resulting distribution tuple can be written as $P_{F(C_x),D_y}(a,b)$ where the self-map $F$ on $A$ is given by $F(a) = a$ for $a \not\in A'$ and $F(a) = a'$ for $a \in A'$. Consequently, the component for the inputs $x$ and $y$ and outputs $a$ and $b$ of $T_k(P)$ in eq. (B1) can be expressed as $P_{F_x,k(A_x(x,k)),G_{y,k}(B_{t(y,k)})(a,b)}$ with self-maps $F_x,k$ and $G_{y,k}$ on $A$ and $B$, respectively, determined by $O_A^k$ and $O_B^k$, respectively.

The above shows that

$$P_{x,y}' = \rho_0 P_{\tilde{A},\tilde{B}} + \sum_{k \geq 1} \rho_k P_{F_x,k(A_x(x,k),G_{y,k}(B_{t(y,k)})(a,b))}.$$  

It remains to introduce a random non-negative integer $K$ with distribution $P_k(K) = p_k$ and the random variables $A'_x$ and $B'_y$ given in the Lemma. The probability mass function of $K$, $A'_x$ and $B'_y$ is $P_{F_x,k(A_x(x,k)),G_{y,k}(B_{t(y,k)})(a,b)}$ with

$$P_{A'_x,B'_y|K}(a,b|k) = P_{F_x,k(A_x(x,k)),G_{y,k}(B_{t(y,k)})(a,b)}$$

for a quantum $P$, the distributions of the $A_x$ and $B_y$ can be written as

$$P_{A_x,B_y}(a,b) = \rho(M_{x,a} \otimes N_{y,b})$$

where $\rho_{lu}$ is a density operator on $H_A \otimes H_B$ and $M_{x,a}$ and $N_{y,b}$ are positive operators such that $\sum_{a,e} M_{x,a} = I_A$ and $\sum_{b,e} N_{y,b} = I_B$. For any self-maps $F$ on $A$ and $G$ on $B$, one has

$$P_{F(A_x),G(B_y)}(a,b) = \sum_{a',b',t} P_{A_x,B_y}(a',b').$$

This expression can be recast into the form of eq. (B2) with $M_{x,a}$ and $N_{y,b}$ replaced, respectively, by the operators $M_{x,a}$ and $N_{y,b}$ defined similarly and so

$$P_{F_{x,k}(A_x(x,k)),G_{y,k}(B_{t(y,k)})(a,b)} = \rho_{lu} M_{F_{x,k}(x,k),a} \otimes N_{G_{y,k}(t,y(k),b)}.$$  

The Bell local distribution tuple $L$ is also given by eq. (B2) with $\rho_{lu}$, $M_{x,a}$ and $N_{y,b}$ replaced by

$$\rho'_{lu} = \sum_{k,a,b} P(k) P_{A,B}(a,b) \Pi_{A_x,B_y}^{k,a,b} \otimes \Pi_{A_x,B_y}^{k,a,b},$$

with the same notations as in eq. (B3). The sum of the projectors $\Pi_{A_x,B_y}^{k,a,b}$, respectively, is the identity operator on a Hilbert space $H_A \otimes H_B$, $H_A \otimes H_B$. Alice and Bob then

$$M_{x,a} = \sum_{k,a,b} \Pi_{A_x,a,b} \delta_{k,a} \Pi_{A_x,a,b} \otimes \Pi_{A_x,a,b} \otimes \Pi_{A_x,a,b},$$

and $N_{y,b}$ defined similarly, leads to $P'$, which is hence quantum.

**Appendix C: Proof of Proposition 1**

(i) Let $P$ and $P'$ be two quantum distribution tuples with numbers $m$ and $n$ of inputs such that the former is not less nonlocal than the latter. For these tuples, the Lemma gives the random variables $K_x, A'$ and $B'_y$ for $a_x \in A'$ and $a' \in A'$. Consequently, the component for the inputs $x$ and $y$ and outputs $a$ and $b$ of $T_k(P)$ in eq. (B1) can be expressed as $P_{F_x,k(A_x(x,k)),G_{y,k}(B_{t(y,k)})(a,b)}$ with self-maps $F_x,k$ and $G_{y,k}$ on $A$ and $B$, respectively, determined by $O_A^k$ and $O_B^k$, respectively.

The above shows that

$$P_{x,y}' = \rho_0 P_{\tilde{A},\tilde{B}} + \sum_{k \geq 1} \rho_k P_{F_x,k(A_x(x,k)),G_{y,k}(B_{t(y,k)})(a,b)}.$$  

Finally, equation (B2) with $\rho_{lu}$, $M_{x,a}$ and $N_{y,b}$ replaced by $\rho_{lu} \otimes \rho_{lu}$.

$$M_{x,a} = \sum_{k,a,b} \Pi_{A_x,a,b} \delta_{k,a} \Pi_{A_x,a,b} \otimes \Pi_{A_x,a,b} \otimes \Pi_{A_x,a,b},$$

and $N_{y,b}$ defined similarly, leads to $P'$, which is hence quantum.
generate $U$ and $V$ according to $rkp'$ and discard $X'$, $U'$, $Y'$, $V'$, $K$, the $A_x$ and the $B_y$, which leads to

$$
\omega = \sum_{a,b,x,y} P_{A,B}(a,b)O_{x,y} \otimes \left[ p_0 \Pi_{az,by}^{U,V} \otimes \Pi_{,a,b}^{E_{Ev}} \otimes \text{tr}_H \rho \right] + \sum_{k \geq 1} p_k \Pi_{X,k}^{U,V} \otimes \Pi_{,a,b}^{E_{Ev}} \otimes \text{tr}_H (\rho M_{x,k}(u') \otimes N_{y,(k),v'} \otimes I_E),
$$

where $x$ and $y$ correspond to $X$ and $Y$, respectively, $\Pi_{U,V}^{x,y}$ denotes mutually orthogonal rank-one projectors and the notations $O_{x,y} = \sum_e P_{X,Y,E}(x,y,e)\Pi_{x,e}^{A_{Alice}} \otimes \Pi_{y,e}^{B_{Bob}} \otimes \Pi_{E_{Ev}}$, $p_k = P_k(k)$ and $H = H_A \otimes H_B$ are used. The state $\omega$ can be rewritten as

$$
\omega = \sum_{x,y,u,v} O_{x,y} \otimes \Pi_{U,V}^{x,y} \otimes \text{tr}_H (((\rho' \otimes \rho)(M_{x,u}^{I} \otimes N_{y,v}^{I} \otimes I_E))),
$$

where $M_{x,u}^{I}$ is given by eq. (14), $N_{y,v}^{I}$ by a similar expression, $\Pi_{I}^{E_{Ev}}$ is the identity operator on $H_E \otimes H'^{E_{Ev}}$ and $H' = H_A \otimes H'^{A_{Alice}} \otimes H_B \otimes H'^{B_{Bob}}$. As soon as $\text{tr}(\rho M_{x,a}^{I} \otimes N_{y,b}^{I} \otimes I_E) = P_{x,y}(a,b)$, the state $\rho' \otimes \rho$, the operators $M_{x,a}^{I}$ and $N_{y,b}^{I}$ given by eq. (14) and the distributions $P_{x,y}$ are related in the same way, see the proof of the Lemma. Thus, one has $R(\rho') \leq S'$ where $S'$ is defined similarly as $R(\rho)$ but taking the infimum only over such particular states and measurement operators. When the state initially shared by the three parties is $\rho' \otimes \rho$ and Alice’s and Bob’s measurements are characterized by the operators $M_{x,a}^{I}$ and $N_{y,b}^{I}$, respectively, performing $rkp_1$ and generating $U$ and $V'$ according to $rkp'$ gives the state (C2), see the derivation of equation (3). So, in this case, the tripartite state obtained at the end of $rkp$ is identical to that resulting from the execution of the protocol $rkp'$ with $\rho$, $M_{x,a}^{I}$ and $N_{y,b}^{I}$. Consequently, $S$ and $S'$ are equal to each other, which finishes the proof of property (i).

(ii) Any Bell local distribution tuple can be written in quantum form with the state given by eq. (C1) without $K$ and measurement operators $\sum_{a,b} \delta_{a,b} \Pi_{x,y}^{A_{Alice}}$ and $\sum_{a,b} \delta_{b,a} \Pi_{x,y}^{B_{Bob}}$, see the proof of the Lemma. Performing any raw key protocol with this initial state and Alice’s and Bob’s measurements described by these operators leads to the state

$$
\rho_{r_k} = \sum_{a,b,x,y} P_{A,U,X,E}(a|x,e)P_{B|V,Y,E}(b|y,e) \otimes P_{X,Y,E}(x,y,e)P_{A,B}(a,b) \Pi_{x,y} \otimes \Pi_{y,b} \otimes \Pi_{x,a,b},
$$

where $x$ ($y$) corresponds to $X$ ($Y$) and $\Pi_{x,a,b} = \Pi^{E_{Ev}} \otimes \Pi^{x,y,a,b}$. Assume that Eve simply makes the measurement of operators $\Pi_{x,a,b}$ on $\rho_{r_k}$. The three parties are left with classical random variables. Since $P_{X,Y,E} = P_{X,E}P_{Y,E}P_E$, the probability mass function of $A$, $B$ and the random variables available to Eve, i.e., $A$, $B$ and $E$, is $P_{A,E}P_{B,E}P_{E}$ and hence $A$ and $B$ are conditionally independent given Eve’s variables. Consequently, Alice and Bob cannot generate a secret key [25].

### Appendix D: Proof of Proposition 2

For any $P \in Q$, we define the family of distribution tuples $P_p = pP + (1 - p)L$ where $L$ is any Bell local distribution tuple and $p$ varies from 0 to 1. They belong to $Q$ since $\mathcal{L} \subset Q$ and $Q$ is convex [25]. Clearly, $P_p$ is continuous with respect to $p$, $P_1 = P$ and $P_0 = L$. Moreover, $P$ is not less nonlocal than $P_p$ for any $p \in [0,1]$. We denote by $Q_s$ the set of all $P \in Q$ such that $N(P) = s$ and define the function $f$, on the set $I$ of the values of $N$, by $f(s) = \inf_{P \in Q} M(P)$. By construction, $f \circ N \leq M$ on $Q$ and there is, for any $s \in I$, $P \in Q_s$ such that $M(P) = f(s)$ and $f(s)$ are as close to each other as we wish. Since $M$ and $N$ vanish on $\mathcal{L}$, there is a set $Q_0$ containing $\mathcal{L}$ and $f(0) = 0$.

The set $Q$ is closed and bounded [25] and so, due to the extreme value theorem, the continuous function $N$ has a maximum on $Q$. It is nonnegative since $N$ is. We name it as $N_m$. Consider $\hat{P} \in Q$ such that $N(\hat{P}) = N_m$, and define $\hat{P}_p$ as described above. Owing to the continuity properties of $N$ and $\hat{P}_p$, $N(\hat{P}_p)$ is a continuous function of $p$. It is equal to 0 for $p = 0$ and to $N_m$ for $p = 1$. Thus, due to the intermediate value theorem, for any $s \in [0,N_m]$, there is $q$ such that $N(\hat{P}_q) = s$. Consequently, $I$ is equal to this interval.

For any $P \in Q_s$, $N(P_p)$ is a continuous function of $p$ which is equal to 0 for $p = 0$ and to $s$ for $p = 1$. So, for any $s' \in [0,s]$, there is $q$ such that $P_q \in Q_{s'}$. Moreover, since $P$ is not less nonlocal than $P_q$ and $M$ is a nonlocality monotone, one has $M(P) \geq M(P_q)$ for $s'$. Thus, for any $s$ and $s'$ in $I$ such that $s' \leq s$, $f(s')$ is a lower bound of $M$ on $Q_s$, which implies that $f$ is nondecreasing.

### Appendix E: Upper Bound on the threshold $\hat{N}^*$

The largest rate $R'(\rho_{r_k})$ at which Alice and Bob can establish a common private key when they share a large number of copies of the state $\rho_{r_k}$, given by eq.(3) in the main text, with Eve obeys

$$
R'(\rho_{r_k}) \geq I(A : B) + \sum_{a} P_A(a)S(\omega_a) - S(\omega),
$$

where $I(A : B)$ is the mutual information between $A$ and $B$, $S$ denotes the von Neumann entropy, $\omega = \text{tr}_{H_{AB}} \rho'$ and $\omega_a = \text{tr}_{H_{AB}} (\rho' M_a \otimes I_B \otimes I_E)/P_A(a)$ with $I_E$ the identity operator on $H_B \otimes H'^{B}_{Bob}$ [8]. We consider $m = n = 2$, random variables $A_z$ and $B_y$ with values in $\{0,1\}$ and a raw key protocol in which Alice creates three equally distributed random variables, $X$, $Y$ and $Z$ and sends $Y$ and $Z$ over the public channel, $\nu = \nu(X,Y)ZU$ where $\nu$ is a map from $\{1,2\}$ to $\{-1,1\}$ such that $\nu(x,y) =$
−1 for only one pair \((x, y)\) and \(B = ZV\). The values of \(Z\) are \(-1\) and 1, \(X\) and \(Y\) are the choice random variables for Alice and Bob, respectively, with alphabet \([1, 2]\). Consequently, \(P_A = P_B = 1/2\) and the above Eve’s states are given by
\[
\omega = \sum_{y,z} \Pi_{y,z} \otimes \text{tr}_{H_A \otimes H_B} \rho/4
\]
and
\[
\omega_a = \sum_{x,y,z} \Pi_{y,z} \otimes \text{tr}_{H_A \otimes H_B} (\rho M_{x,z} v(x,y) a \otimes I_B \otimes I_E)/4,
\]
omitting the superscript for the projectors.

Since \(m = n = 2\) and \(A = B = \{-1, 1\}\), these states can be rewritten as
\[
\omega = \sum_{y,z} \lambda \Pi_{y,z} \otimes \text{tr}_{H_A} \rho_A/4
\]
and
\[
\omega_a = \sum_{x,y,z} \frac{p_A}{8} \Pi_{y,z} \otimes \text{tr}_{H_A} \rho_A (I + z \nu a \Sigma_{x,z}^A) \otimes I \otimes I_E,
\]
omitting the arguments of \(\nu\), where \(p_A\) denotes probabilities summing to unity, \(\mathcal{H}\) the Hilbert space of dimension 2, \(\rho_A\) density operators on \(\mathcal{H}^2 \otimes \mathcal{H}_E\), and \(I\) the identity operator on \(\mathcal{H}\). In some basis of \(\mathcal{H}\), depending on \(\lambda\), the diagonal elements of the operators \(\Sigma_{x,z}^A\) can be expressed as \(\pm \cos \theta_{x,z,\lambda}\) and the nondiagonal ones as \(\sin \theta_{x,z,\lambda}\) [9]. In terms of the states \(\rho_A\), the distributions \(P_{x,y}\) read as
\[
P_{x,y}(a, b) = \sum_a \frac{p_A}{4} \text{tr}(\rho_A (I + a \Sigma_{x,z}^A) \otimes (I + b \Sigma_{y,z}^B) \otimes I_E),
\]
where the operators \(\Sigma_{y,z}^B\) are similar to the \(\Sigma_{x,z}^A\).

The above Eve’s states can be further simplified into
\[
\omega = \sum_{\lambda} \lambda p_A \text{tr}_{H_A} \rho'_A\]
and
\[
\omega_a = \sum_{x,y,z} \frac{p_A}{2} \text{tr}_{H_A} \rho'_A (I + a \Sigma_{x,z}^A) \otimes I \otimes I_E).
\]
The states \(\rho'_A\) are given by
\[
\rho'_A = \sum_{y,z} \Pi_{y,z} \otimes \rho_{y,z}/4
\]
where \(\rho_{x,z} = \rho_A\) and \(\rho_{x,-z} = -\sigma_A^x \otimes \sigma_B^z \otimes I_E\rho_A \sigma_A^x \otimes \sigma_B^z \otimes I_E\) with \(\sigma_A^x = (0 \ 1 \ 1 \ 0)\) in the basis in which the \(\Sigma_{x,z}^A\) are real and similarly for \(\sigma_B^z\). The above expression for \(\omega_a\) results from \(\sigma_A^x \Sigma_{x,z}^A \sigma_A^x = -\Sigma_{x,z}^A\) and the reduced density operator on \(\mathcal{H}^2\) of \(\rho'_A\) is \(\text{tr}_{H_E} (\rho_{x,z} + \rho_{x,-z}/2\) which can always be taken to be a Bell diagonal state and hence
\[
S(\omega_A) - \sum_a S(\omega_{A,x,a})/2 \leq h([1 + (N_A + N_B^2)/4]/2)/2,
\]
where \(\omega_A = \text{tr}_{H_A} \rho'_A\), \(\omega_{A,x,a} = \text{tr}_{H_A} \rho'_A (I + a \Sigma_{x,z}^A) \otimes I \otimes I_E), h\) is the binary entropy function and \(N_A\) is the maximum violation of the Clauser-Horne-Shimony-Holt inequality [29] for the state \(\text{tr}_{H_E} (\rho_{x,z} + \rho_{x,-z}/2\) [9]. As \(\sum_a ab P_{x,y}(a, b) = \sum_{a,b} ab P_{x,y}(-a, -b)\), the value of \(\langle A_x B_y \rangle\) remains the same when \(\rho_A\) is replaced by \((\rho_{x,z} + \rho_{x,-z}/2\) and so \(N(P) \leq \sum_{a,b} p_A N_{a,b}\) where \(N\) is defined by eq.(7) in the main text. Thus, due to the properties of the Holevo quantity and of \(h\), the above inequality is valid with \(\omega_A\), \(\omega_{A,x,a}\) and \(N_A\) replaced, respectively, by \(\omega_a\), \(\omega_{a,x,a}\) and \(N(P)\).

Since \(P_A = P_B = 1/2\), one has \(I(A : B) = 1 - h(1/2 + |\langle AB \rangle|)/2\) where
\[
\langle AB \rangle = \langle \nu(X, Y)UV \rangle = \frac{1}{4} \sum_{x,y} \nu(x,y) \langle A_x B_y \rangle,
\]
and thus \(\max_a I(A : B) \geq 1 - h(3/4 + \tilde{N}(P)/8).\) The above results show that \(R \geq g' \circ \tilde{N}\) where \(g'\) is given by
\[
g'(z) = 1 - h \left( \frac{3}{4} + \frac{z}{8} \right) - h \left( \frac{1}{2} + \frac{1}{2} \sqrt{z + \frac{z^2}{4}} \right).
\]
As \(R\) is nonnegative, the right side of the above inequality can be replaced by zero when it is negative and hence \(R \geq g \circ \tilde{N}\) with \(g(z) = \max\{0, g'(z)\}\). The value \(g'(z)\) is positive for \(z \geq 0.652\). So, the nonlocality monotone \(N\) has a threshold value \(N^* \leq 0.652\).

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