

Third-order Analysis of Channel Coding in the Moderate Deviations Regime

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Abstract—The channel coding problem in the moderate deviations regime is studied; here, the error probability decays sub-exponentially to zero, and the rate approaches the capacity slower than $O(1/\sqrt{n})$. Our result refines Altuğ and Wagner’s moderate deviations result by deriving lower and upper bounds on the third-order term in the asymptotic expansion of the maximum achievable message set size. The third-order term of our expansion employs a new quantity here called the channel skewness. For the binary symmetric channel and most practically important (n, ϵ) pairs, including $n \in [100, 500]$ and $\epsilon \in [10^{-10}, 10^{-1}]$, an approximation up to the channel skewness is the most accurate among several expansions in the literature.

I. INTRODUCTION

The fundamental limit of channel coding is the maximum achievable message set size $M^*(n, \epsilon)$ given a channel $P_{Y|X}$, a blocklength n , and an average error probability ϵ . Since determining $M^*(n, \epsilon)$ exactly is difficult for arbitrary triples $(P_{Y|X}, n, \epsilon)$, the literature investigating the behavior of $M^*(n, \epsilon)$ studies two asymptotic regimes: the central limit theorem (CLT) and large deviations (LD) regimes. To make this precise, consider the sum of n independent and identically distributed (i.i.d.) random variables. By the CLT, the probability that this sum deviates from the mean by order- \sqrt{n} is characterized by the Gaussian distribution, whose parameters are constant with respect to n . By Cramér’s theorem [1], commonly known as the LD theorem, the probability that the sum of n i.i.d. random variables deviates from the mean by order- n decays exponentially with n if Cramér’s condition is satisfied. Deviations from the mean by order strictly greater than \sqrt{n} and strictly smaller than n are called moderate deviations (MD). Bounds on the probability with which an i.i.d. sum deviates from the mean by an amount that falls in the MD regime are given in [2, Ch. 8]. This work focuses on channel coding in the MD regime.

Given a channel, error probability ϵ , and blocklength n , we define the *non-Gaussianity* of a channel, which captures the third-order term in a rate characterization, as

$$\zeta(n, \epsilon) \triangleq \log M^*(n, \epsilon) - (nC - \sqrt{nV_\epsilon}Q^{-1}(\epsilon)), \quad (1)$$

where C is the capacity, and $V_\epsilon > 0$ is the ϵ -dispersion of the channel [3, Sec. IV].

Channel coding analyses in the CLT regime fix a target error probability $\epsilon \in (0, 1)$ and approximate $M^*(n, \epsilon)$ as the

blocklength n approaches infinity by the bracketed term in (1). Examples of such results include Strassen’s results [4] for discrete memoryless channels (DMCs) under the maximal error probability constraint with $\zeta(n, \epsilon) = O(\log n)$. Polyanskiy *et al.* [3] and Hayashi [5] revisit Strassen’s result [4], showing that the same asymptotic expansion holds for the average error probability constraint, deriving lower and upper bounds on the coefficient of the $\log n$ term, and extending the result to the Gaussian channel with maximal and average power constraints. CLT-style analyses also exist for channels with feedback [6], lossy [7] and lossless data compression [4], [8], network information theory [9], random access channels [10], [11], and many other scenarios.

For channel coding in the LD regime, which is commonly known as the error exponent regime, one fixes a rate $R = \frac{\log M}{n}$ strictly below the channel capacity and seeks to characterize the minimum achievable error probability $\epsilon^*(n, R)$ as the blocklength n approaches infinity. In this regime, $\epsilon^*(n, R)$ decays exponentially with n , and [12, Ch. 5] derives the optimal error exponent $\lim_{n \rightarrow \infty} -\frac{1}{n} \log \epsilon^*(n, R)$ for R above the critical rate.

In [13], Altuğ and Wagner seek to bridge the gap between the CLT and LD regimes. In their asymptotic regime, the error probability ϵ_n decays sub-exponentially to zero, i.e., $\epsilon_n \rightarrow 0$ and $-\frac{1}{n} \log \epsilon_n \rightarrow 0$, and the rate approaches the capacity with a gap of order strictly greater than $\frac{1}{\sqrt{n}}$. Altuğ and Wagner argue that this formulation is more practically relevant since it simultaneously considers low error probabilities and high achievable rates. For DMCs with positive ϵ_n -dispersion V_{ϵ_n} and a sequence of sub-exponentially decaying ϵ_n , they show that

$$\zeta(n, \epsilon_n) = o(\sqrt{n}V_{\epsilon_n}Q^{-1}(\epsilon_n)). \quad (2)$$

This result implies that the dispersion approximation to the maximum achievable message set size $\log M^*(n, \epsilon_n) \approx nC - \sqrt{nV_{\epsilon_n}}Q^{-1}(\epsilon_n)$, as in (1) is still valid in the MD regime; however, they do not specify how accurate it is since they do not derive the leading term of $\zeta(n, \epsilon_n)$. Our goal is to determine the accuracy of the dispersion approximation in this regime by deriving tight bounds on the non-Gaussianity. In [14], Polyanskiy and Verdú give an alternative proof of (2) and extend the result to the Gaussian channel with a maximal power constraint. In [15], Chubb *et al.* extend the second-order result in (2) to quantum channels.

Emerging applications with tight delay constraints motivate interest in refining the asymptotic expansions of maximum achievable channel coding rate. For small blocklength n , the non-Gaussianity $\zeta(n, \epsilon)$ in (1) can be quite large when

compared to the second-order term $O(\sqrt{n})$. For example, in the CLT regime, given a DMC with finite input alphabet \mathcal{X} and output alphabet \mathcal{Y} , [3] bounds the non-Gaussianity as

$$O(1) \leq \zeta(n, \epsilon) \leq \left(|\mathcal{X}| - \frac{1}{2} \right) \log n + O(1). \quad (3)$$

A variety of refinements follow. The first considers non-singular channels, where singular channels are channels for which the channel transition probability from x to y is the same for every compatible (x, y) pair, while nonsingular channels are channels that do not satisfy this property; see Section II-E for formal definitions. For nonsingular channels, the random coding union bound improves the lower bound to $\frac{1}{2} \log n + O(1)$ [16, Cor. 54]. For DMCs with positive ϵ -dispersion, Tomamichel and Tan [17] improve the upper bound to $\frac{1}{2} \log n + O(1)$. A random variable is called lattice if it takes values on a lattice with probability 1, and is called non-lattice otherwise. For nonsingular channels with positive ϵ -dispersion and non-lattice information density, Moulin [18] shows

$$\zeta(n, \epsilon) \geq \frac{1}{2} \log n + \underline{S} Q^{-1}(\epsilon)^2 + \underline{B} + o(1) \quad (4)$$

$$\zeta(n, \epsilon) \leq \frac{1}{2} \log n + \overline{S} Q^{-1}(\epsilon)^2 + \overline{B} + o(1), \quad (5)$$

where \underline{S} , \overline{S} , \underline{B} , and \overline{B} are constants depending on the channel parameters. Gallager-symmetric channels are channels for which the output alphabet can be partitioned into subsets in a way that for each subset of the probability transition matrix that uses inputs as rows and outputs of the subset as columns has the property that each row (respectively column) is a permutation of each other [12, p. 94]. For Gallager-symmetric, singular channels, $\zeta(n, \epsilon) = O(1)$ [19]. Bounds on the sub-exponential factors in the LD regime for singular and nonsingular channels appear in [19]–[22].

In this work, we extend the definition of the MD error probability region in [13] to include the sequences that sub-exponentially approach 1 or other constant values: we say that a sequence of error probabilities $\{\epsilon_n\}_{n=1}^{\infty}$ is an MD sequence if for all $c > 0$, there exists some $n_0 \in \mathbb{N}$ such that

$$\exp\{-cn\} \leq \epsilon_n \leq 1 - \exp\{-cn\} \quad (6)$$

for all $n \geq n_0$. We refine the lower and upper bounds in (2) for nonsingular channels. Our result generalizes (4)–(5) to all error probability sequences ϵ_n satisfying (6) at the expense of not bounding the constant term. We show that for nonsingular channels with positive minimum dispersion and ϵ_n satisfying (6), $\zeta(n, \epsilon_n)$ in (2) satisfies the following bounds from below and above as

$$\frac{1}{2} \log n + \underline{S} Q^{-1}(\epsilon_n)^2 + O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right) + O(1) \leq \zeta(n, \epsilon_n) \quad (7)$$

$$\leq \frac{1}{2} \log n + \overline{S} Q^{-1}(\epsilon_n)^2 + O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right) + O(1), \quad (8)$$

where the constants \underline{S} and \overline{S} are the same as in (4) and (5). We show that the non-Gaussianity approaches $O(\sqrt{n})$ as ϵ_n approaches an exponential decay, rivaling the dispersion term in (1). Thus, refining the third-order term as we do in (7)–(8)

is especially important in the MD regime. Our achievability bound applies the standard random coding bound used in both the CLT [3], [18] and LD [20] regimes. Our converse bound combines the result in [17, Prop. 6], which is a relaxation of the meta-converse bound [3, Th. 27], and a saddlepoint result of a minimax problem in [18, Lemma 14]. Neither the Berry-Esseen theorem used in [3] nor the refined Edgeworth expansion used in [18] to treat the constant ϵ case is sharp enough for the $O(1)$ precision in (7)–(8), which applies to any sequence ϵ_n satisfying (6). We replace these tools with the moderate deviations bounds found in [2, Ch. 8].

We define the channel *skewness* operationally as

$$S \triangleq \lim_{\epsilon \rightarrow 0} \limsup_{n \rightarrow \infty} \frac{\zeta(n, \epsilon) - \frac{1}{2} \log n}{Q^{-1}(\epsilon)^2}. \quad (9)$$

For the maximum achievable rate, the channel skewness characterizes third-order bounds much like channel dispersion characterizes second-order bounds in [3, Sec. IV]. The quantities \underline{S} and \overline{S} provide informational lower and upper bounds to the channel skewness. They depend on the second and third moments of the information density under a dispersion-achieving input distribution.

For Cover-Thomas symmetric channels [23], where each row (respectively column) of the probability transition matrix is a permutation of each other, $\underline{S} = \overline{S}$. For the binary symmetric channel (BSC) and a wide range of (n, ϵ) pairs, our asymptotic approximation for the maximum achievable rate using terms up to the channel skewness, i.e., $\zeta(n, \epsilon) \approx \frac{1}{2} \log n + S Q^{-1}(\epsilon)^2$ is more accurate than both Moulin's bounds with \underline{B} and \overline{B} in (4) and (5) included and the normal approximation, which takes $\zeta(n, \epsilon) \approx \frac{1}{2} \log n$; our approximation competes with the saddlepoint approximations in [21], [22]. Moreover, for the BSC with an (n, ϵ) pair satisfying $\epsilon \in [10^{-10}, 10^{-1}]$ and $n \in [100, 500]$, including the leading term of $O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right)$ in our approximation (see Section VI) yields a less accurate approximation than is obtained by stopping at the channel skewness. This highlights the importance of channel skewness relative to the higher-order terms in characterizing the channel. Characterization of all $(P_{Y|X}, n, \epsilon)$ triples satisfying this property remains an open problem.

Using the moderate deviations results in [2, Ch. 8] and the strong large deviations results in [24], we derive the asymptotics of binary hypothesis testing in the MD regime (Theorem 6), characterizing the minimum achievable type-II error of a hypothesis test that chooses between two product distributions (i.e., the β_α function defined in [3]), given that type-I error is an MD sequence (6). Binary hypothesis testing is known to be closely related to several information-theoretic problems. For instance, Blahut [25] derives a lower bound on the error exponent in channel coding in terms of the asymptotics of binary hypothesis testing in the LD regime. Polyanskiy *et al.* derive a converse result [3, Th. 27] in channel coding using the minimax of the β_α function; this converse is commonly known as the meta-converse bound. Kostina and Verdú prove a converse result for fixed-length lossy [7, Th. 8] compression of stationary memoryless sources using the β_α function. This result is extended to lossless joint

source-channel coding in [26]. For lossless data compression, Kostina and Verdú give lower and upper bounds [7, eq. (64)] on the minimum achievable codebook size in terms of β_α . For lossless multiple access source coding, also known as Slepian-Wolf coding, Chen *et al.* derive a converse result [27, Th. 19] in terms of the composite hypothesis testing version of the β_α function that considers a single null hypothesis and k alternative hypotheses. Composite hypothesis testing is also used in a random access channel coding scenario to decide whether any transmitter is active [11]. The works in [3], [7], [11], [26], [27] derive second- or third-order asymptotic expansions for their respective problems by using the asymptotics of the β_α function in the CLT regime. As an application of Theorem 6, the results in [3], [7], [11], [26], [27] could be extended to the MD regime. For Cover-Thomas symmetric channels, we show a refined converse result in Theorem 8 using Theorem 6 and the meta-converse bound.

The paper is organized as follows. We define notation and give the preliminaries to present our results in Section II. Section III presents and discusses the main results. Proofs of the main results appear in Section IV. The asymptotics of binary hypothesis testing in the MD regime are derived in Section V. Refined bounds for Cover-Thomas symmetric channels appear in Section VI.

II. NOTATION AND PRELIMINARIES

A. Notation

For any $k \in \mathbb{N}$, we denote $[k] \triangleq \{1, \dots, k\}$. We denote random variables by capital letters (e.g., X) and individual realizations of random variables by lowercase letters (e.g., x). We use boldface letters (e.g., \mathbf{x}) to denote vectors, calligraphic letters (e.g., \mathcal{X}) to denote alphabets and sets, and sans serif font (e.g., \mathbf{A}) to denote matrices. The i -th entry of a vector \mathbf{x} is denoted by x_i , and (i, j) -th entry of a matrix \mathbf{A} is denoted by $A_{i,j}$. The sets of real numbers and complex numbers are denoted by \mathbb{R} and \mathbb{C} , respectively. All-zero and all-one vectors are denoted by $\mathbf{0}$ and $\mathbf{1}$, respectively. A vector inequality $\mathbf{x} \leq \mathbf{y}$ for $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ is understood element-wise, i.e., $x_i \leq y_i$ for all $i \in [d]$. We denote the inner product $\sum_{i=1}^d x_i y_i$ by $\langle \mathbf{x}, \mathbf{y} \rangle$. We use $\|\cdot\|$ to denote the ℓ_∞ norm, i.e., $\|\mathbf{x}\| \triangleq \max_{i \in [d]} |x_i|$.

The sets of all distributions on the channel input alphabet \mathcal{X} and the channel output alphabet \mathcal{Y} are denoted by \mathcal{P} and \mathcal{Q} , respectively. We write $X \sim P_X$ to indicate that X is distributed according to $P_X \in \mathcal{P}$. Given a distribution $P_X \in \mathcal{P}$ and a conditional distribution $P_{Y|X}$ from \mathcal{X} to \mathcal{Y} , we write $P_X \times P_{Y|X}$ to denote the joint distribution of (X, Y) , and P_Y to denote the marginal distribution of Y , i.e., $P_Y(y) = \sum_{x \in \mathcal{X}} P_X(x) P_{Y|X}(y|x)$ for all $y \in \mathcal{Y}$. Given a conditional distribution $P_{Y|X}$, the distribution of Y given $X = x$ is denoted by $P_{Y|X=x}$. The skewness of a random variable X is denoted by $\text{Sk}(X) \triangleq \frac{\mathbb{E}[X^3]}{\text{Var}[X]^{3/2}}$. For a sequence $\mathbf{x} = (x_1, \dots, x_n)$, the empirical distribution (or type) of \mathbf{x} is denoted by

$$\hat{P}_{\mathbf{x}}(x) = \frac{1}{n} \sum_{i=1}^n \mathbf{1}\{x_i = x\}, \quad \forall x \in \mathcal{X}. \quad (10)$$

A lattice random variable is a random variable taking values in $\{a + kd : k \in \mathbb{Z}\}$, where d is the *span* of the lattice. We say that a random vector $\mathbf{X} = (X_1, \dots, X_n)$ is non-lattice if each of X_i , $i \in [n]$ is non-lattice, and is lattice if each of X_i , $i \in [n]$ is lattice.¹ We measure information in nats, and logarithms and exponents have base e .

As is standard, $f(n) = O(g(n))$ means $\limsup_{n \rightarrow \infty} \left| \frac{f(n)}{g(n)} \right| < \infty$, and $f(n) = o(g(n))$ means $\lim_{n \rightarrow \infty} \left| \frac{f(n)}{g(n)} \right| = 0$. We use $Q(\cdot)$ to represent the complementary Gaussian cumulative distribution function $Q(x) \triangleq \frac{1}{\sqrt{2\pi}} \int_x^\infty \exp\left\{-\frac{t^2}{2}\right\} dt$ and $Q^{-1}(\cdot)$ to represent its functional inverse.

B. Definitions related to information density

The relative entropy, divergence variance, and divergence centralized third moment between distributions P and Q on a common alphabet are denoted by

$$D(P\|Q) \triangleq \mathbb{E} \left[\log \frac{P(X)}{Q(X)} \right] \quad (11)$$

$$V(P\|Q) \triangleq \text{Var} \left[\log \frac{P(X)}{Q(X)} \right] \quad (12)$$

$$T(P\|Q) \triangleq \mathbb{E} \left[\left(\log \frac{P(X)}{Q(X)} - D(P\|Q) \right)^3 \right], \quad (13)$$

where $X \sim P$. Let $P_X \in \mathcal{P}$, $Q_Y \in \mathcal{Q}$, and $P_{Y|X}$ be a conditional distribution from \mathcal{X} to \mathcal{Y} . The conditional relative entropy, conditional divergence variance, conditional divergence centralized third moment, and conditional divergence skewness are denoted by

$$D(P_{Y|X}\|Q_Y|P_X) \triangleq \sum_{x \in \mathcal{X}} P_X(x) D(P_{Y|X=x}\|Q_Y) \quad (14)$$

$$V(P_{Y|X}\|Q_Y|P_X) \triangleq \sum_{x \in \mathcal{X}} P_X(x) V(P_{Y|X=x}\|Q_Y) \quad (15)$$

$$T(P_{Y|X}\|Q_Y|P_X) \triangleq \sum_{x \in \mathcal{X}} P_X(x) T(P_{Y|X=x}\|Q_Y) \quad (16)$$

$$\text{Sk}(P_{Y|X}\|Q_Y|P_X) \triangleq \frac{T(P_{Y|X}\|Q_Y|P_X)}{V(P_{Y|X}\|Q_Y|P_X)^{3/2}}. \quad (17)$$

Let $(X, Y) \sim P_X \times P_{Y|X}$. The information density is defined as

$$i(x; y) \triangleq \log \frac{P_{Y|X}(y|x)}{P_Y(y)}, \quad \forall x \in \mathcal{X}, y \in \mathcal{Y}. \quad (18)$$

We define the following moments of the random variable $i(X; Y)$.

- The mutual information

$$I(P_X, P_{Y|X}) \triangleq \mathbb{E}[i(X; Y)] = D(P_{Y|X}\|P_Y|P_X), \quad (19)$$

- the unconditional information variance

$$\begin{aligned} V_u(P_X, P_{Y|X}) &\triangleq V(P_X \times P_{Y|X}\|P_X \times P_Y) \\ &= \text{Var}[i(X; Y)], \end{aligned} \quad (20)$$

¹The case that some of the coordinates of \mathbf{X} are lattice and the rest of its coordinates is non-lattice is excluded in this paper.

- the unconditional information third central moment

$$T_u(P_X, P_{Y|X}) \triangleq T(P_X \times P_{Y|X} \| P_X \times P_Y) \quad (21)$$

$$= \mathbb{E} [(\iota(X; Y) - I(P_X, P_{Y|X}))^3], \quad (22)$$

- the unconditional information skewness

$$\text{Sk}_u(P_X, P_{Y|X}) \triangleq \text{Sk}(\iota(X; Y)) = \frac{T_u(P_X, P_{Y|X})}{V_u(P_X, P_{Y|X})^{3/2}}, \quad (23)$$

- the conditional information variance

$$V(P_X, P_{Y|X}) \triangleq V(P_{Y|X} \| P_Y | P_X) \\ = \mathbb{E} [\text{Var}[\iota(X; Y) | X]], \quad (24)$$

- the conditional information third central moment

$$T(P_X, P_{Y|X}) \triangleq T(P_{Y|X} \| P_Y | P_X), \quad (25)$$

- the conditional information skewness

$$S(P_X, P_{Y|X}) \triangleq \frac{T(P_{Y|X} \| P_Y | P_X)}{V(P_{Y|X} \| P_Y | P_X)^{3/2}}, \quad (26)$$

- the reverse dispersion [16, Sec. 3.4.5]

$$V_r(P_X, P_{Y|X}) \triangleq \mathbb{E} [\text{Var}[\iota(X; Y) | Y]]. \quad (27)$$

C. Discrete memoryless channel

A discrete memoryless channel (DMC) is characterized by a finite input alphabet \mathcal{X} , a finite output alphabet \mathcal{Y} , and a probability transition matrix $P_{Y|X}$, where $P_{Y|X}(y|x)$ is the probability that the output of the channel is $y \in \mathcal{Y}$ given that the input to the channel is $x \in \mathcal{X}$. The input-output relation of a DMC is

$$P_{Y|X}^n(\mathbf{y}|\mathbf{x}) = \prod_{i=1}^n P_{Y|X}(y_i|x_i). \quad (28)$$

We proceed to define the channel code.

Definition 1: An (n, M, ϵ) -code for a DMC $P_{Y|X}$ comprises an encoding function

$$f: [M] \rightarrow \mathcal{X}^n, \quad (29)$$

and a decoding function

$$g: \mathcal{Y}^n \rightarrow [M], \quad (30)$$

that satisfy an average error probability constraint

$$1 - \frac{1}{M} \sum_{m=1}^M P_{Y|X}^n(g^{-1}(m)|f(m)) \leq \epsilon. \quad (31)$$

The maximum achievable message set size $M^*(n, \epsilon)$ under the average error probability criterion is defined as

$$M^*(n, \epsilon) \triangleq \max\{M: \exists \text{ an } (n, M, \epsilon)\text{-code}\}. \quad (32)$$

D. Definitions related to the optimal input distribution

The capacity of a DMC $P_{Y|X}$ is

$$C(P_{Y|X}) \triangleq \max_{P_X \in \mathcal{P}} I(P_X, P_{Y|X}). \quad (33)$$

We denote the set of capacity-achieving input distributions by

$$\mathcal{P}^\dagger \triangleq \{P_X \in \mathcal{P}: I(P_X, P_{Y|X}) = C(P_{Y|X})\}. \quad (34)$$

Even when the capacity-achieving input distribution is not unique ($|\mathcal{P}^\dagger| > 1$), the capacity-achieving output distribution is unique ($P_X, P'_X \in \mathcal{P}^\dagger$ implies $\sum_{x \in \mathcal{X}} P_X(x)P_{Y|X}(y|x) = \sum_{x \in \mathcal{X}} P'_X(x)P_{Y|X}(y|x)$ for all $y \in \mathcal{Y}$) [12, Cor. 2 to Th. 4.5.2]. We denote this unique capacity-achieving output distribution by $Q_Y^* \in \mathcal{Q}$; Q_Y^* satisfies $Q_Y^*(y) > 0$ for all $y \in \mathcal{Y}$ for which there exists $x \in \mathcal{X}$ with $P_{Y|X}(y|x) > 0$ [12, Cor. 1 to Th. 4.5.2]. For any $P_X^\dagger \in \mathcal{P}^\dagger$, it holds that $V(P_X^\dagger, P_{Y|X}) = V_u(P_X^\dagger, P_{Y|X})$ [3, Lemma 62].

Define $V_{\min} \triangleq \min_{P_X^\dagger \in \mathcal{P}^\dagger} V(P_X^\dagger, P_{Y|X})$ and $V_{\max} \triangleq \max_{P_X^\dagger \in \mathcal{P}^\dagger} V(P_X^\dagger, P_{Y|X})$. The ϵ -dispersion [3] of a channel is defined as

$$V_\epsilon \triangleq \begin{cases} V_{\min} & \text{if } \epsilon < \frac{1}{2} \\ V_{\max} & \text{if } \epsilon \geq \frac{1}{2}. \end{cases} \quad (35)$$

The set of dispersion-achieving input distributions is defined as

$$\mathcal{P}^* \triangleq \begin{cases} \{P_X^\dagger \in \mathcal{P}^\dagger: V(P_X^\dagger, P_{Y|X}) = V_\epsilon\} & \text{if } \epsilon \neq \frac{1}{2} \\ \mathcal{P}^\dagger & \text{if } \epsilon = \frac{1}{2}. \end{cases} \quad (36)$$

Any $P_X^\dagger \in \mathcal{P}^\dagger$ satisfies $D(P_{Y|X=x} \| Q_Y^*) = C$ for any $x \in \mathcal{X}$ with $P_X^\dagger(x) > 0$, and $D(P_{Y|X=x} \| Q_Y^*) \leq C$ for all $x \in \mathcal{X}$ [12, Th. 4.5.1]. Hence, the support of any capacity-achieving input distribution is a subset of

$$\mathcal{X}^\dagger = \{x \in \mathcal{X}: D(P_{Y|X=x} \| Q_Y^*) = C\}. \quad (37)$$

The support of any dispersion-achieving input distribution is a subset of

$$\mathcal{X}^* \triangleq \bigcup_{P_X^* \in \mathcal{P}^*} \text{supp}(P_X^*) \subseteq \mathcal{X}^\dagger. \quad (38)$$

The quantities below are used to describe the input distribution that achieves our lower bound \underline{S} on the channel skewness S in (9). The gradient and the Hessian of the mutual information $I(P_X, P_{Y|X})$ with respect to P_X are given by [18]

$$\nabla I(P_X, P_{Y|X})_x = D(P_{Y|X=x} \| P_Y) - 1 \quad (39)$$

$$\nabla^2 I(P_X, P_{Y|X})_{x,x'} = - \sum_{y \in \mathcal{Y}} \frac{P_{Y|X}(y|x)P_{Y|X}(y|x')}{P_Y(y)} \quad (40)$$

for $(x, x') \in \mathcal{X}^2$. The matrix $-\nabla^2 I(P_X^*, P_{Y|X})$ is the same for all $P_X^\dagger \in \mathcal{P}^\dagger$, and is positive semidefinite. See [18, Sec. II-D and II-E] for other properties of $-\nabla^2 I(P_X^\dagger, P_{Y|X})$. Define the $|\mathcal{X}| \times |\mathcal{X}|$ matrix J as

$$J_{x,x'} \triangleq \begin{cases} -\nabla^2 I(P_X^\dagger, P_{Y|X})_{x,x'} & \text{if } x, x' \in \mathcal{X}^\dagger, \\ 0 & \text{otherwise.} \end{cases} \quad (41)$$

Define the set of vectors

$$\mathcal{L} \triangleq \{\mathbf{h} \in \mathbb{R}^{|\mathcal{X}|}: \sum_{x \in \mathcal{X}} h_x = 0, h_{x'} = 0 \text{ for } x' \notin \mathcal{X}^\dagger\},$$

$$h_{x''} \geq 0 \text{ for } x'' \in \mathcal{X}^\dagger \setminus \mathcal{X}^* \}. \quad (42)$$

The following convex optimization problem arises in the optimization of the input distribution achieving the lower bound \underline{S}

$$\sup_{\mathbf{h} \in \mathcal{L} \cap \text{row}(\mathbf{J})} \left(\mathbf{g}^\top \mathbf{h} - \frac{1}{2} \mathbf{h}^\top \mathbf{J} \mathbf{h} \right), \quad (43)$$

where $\text{row}(\cdot)$ denotes the row space of a matrix. If $\mathcal{X}^* = \mathcal{X}^\dagger$, then \mathbf{h} that achieves (43) is given by [18, Lemma 1]

$$\mathbf{h} = \tilde{\mathbf{J}} \mathbf{g}, \quad (44)$$

where

$$\tilde{\mathbf{J}} = \mathbf{J}^+ - \frac{1}{\mathbf{1}^\top \mathbf{J} + \mathbf{1}} (\mathbf{J}^+ \mathbf{1}) (\mathbf{J}^+ \mathbf{1})^\top, \quad (45)$$

\mathbf{J}^+ denotes the Moore-Penrose pseudo-inverse² of \mathbf{J} , and the optimal value in (43) is given by $\frac{1}{2} \mathbf{g}^\top \tilde{\mathbf{J}} \mathbf{g}$.

In our main results, Theorem 1 and Theorem 2 below, we characterize the lower bound \underline{S} and upper bound \bar{S} on the skewness S of the DMC. The following notation is used in those bounds. Define

$$\mathbf{v}(P_X)_x \triangleq \nabla V(P_X, P_{Y|X})_x \quad (46)$$

$$\tilde{\mathbf{v}}_x \triangleq V(P_{Y|X=x} \| Q_Y^*) \quad (47)$$

$$\bar{\mathbf{v}}(P_X)_x \triangleq \mathbb{E} \left[\frac{\partial V(P_{Y|X=x} \| P_Y)}{\partial P_X(x)} \right], \quad x \in \mathcal{X}, \text{ and } X \sim P_X \quad (48)$$

$$A_0(P_X) \triangleq \frac{1}{8V_\epsilon} \mathbf{v}(P_X)^\top \tilde{\mathbf{J}} \mathbf{v}(P_X) \quad (49)$$

$$A_1(P_X) \triangleq \frac{1}{8V_\epsilon} \bar{\mathbf{v}}(P_X)^\top \tilde{\mathbf{J}} \bar{\mathbf{v}}(P_X). \quad (50)$$

See [18, Lemma 2] for properties of these quantities.

E. Singularity of a DMC

The following definition divides DMCs into two groups, for which $M^*(n, \epsilon_n)$ behaves differently in the non-Gaussianity (even in the CLT regime). An input distribution-channel pair $(P_X, P_{Y|X})$ is *singular* [20, Def. 1] if for all (x, \bar{x}, y) such that $P_X \times P_{Y|X}(x, y) > 0$ and $P_X \times P_{Y|X}(\bar{x}, y) > 0$, it holds that

$$P_{Y|X}(y|x) = P_{Y|X}(y|\bar{x}). \quad (51)$$

We define the singularity parameter [18, eq. (2.25)]

$$\eta(P_X, P_{Y|X}) \triangleq 1 - \frac{V_r(P_X, P_{Y|X})}{V_u(P_X, P_{Y|X})}, \quad (52)$$

which is a constant in $[0, 1]$. The pair $(P_X, P_{Y|X})$ is singular if and only if $\eta(P_X, P_{Y|X}) = 1$ [28, Remark 1]. A channel $P_{Y|X}$ is singular if $\eta(P_X^*, P_{Y|X}) = 1$ for all $P_X^* \in \mathcal{P}^*$, and nonsingular otherwise. An example singular channel is the binary erasure channel. Our focus in this paper is on nonsingular channels.

For brevity, if the channel is clear from the context, we drop $P_{Y|X}$ in the notation for capacity, dispersion, skewness, and singularity parameter of the channel.

²Given that $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^\top$ is the singular value decomposition of \mathbf{A} , $\mathbf{A}^+ = \mathbf{V}\Sigma^{-1}\mathbf{U}^\top$.

III. MAIN RESULT

Theorems 1 and 2 are our achievability and converse results, respectively.

Theorem 1: Suppose that ϵ_n satisfies (6) and that $P_{Y|X}$ is a nonsingular DMC with $V_{\epsilon_n} > 0$ for all n and $\mathcal{X}^\dagger = \mathcal{X}^*$. It holds that

$$\zeta(n, \epsilon_n) \geq \frac{1}{2} \log n + \underline{S} Q^{-1}(\epsilon_n)^2 + O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right) + O(1), \quad (53)$$

where

$$\underline{S} \triangleq \max_{P_X^* \in \mathcal{P}^*} \left(\frac{\text{Sk}_u(P_X^*) \sqrt{V_{\epsilon_n}}}{6} + A_0(P_X^*) + \frac{1 - \eta(P_X^*)}{2(1 + \eta(P_X^*))} \right). \quad (54)$$

Proof: The proof consists of two parts and extends the argument in [18]³ to include ϵ_n that decreases to 0 or increases to 1 as permitted by (6). The first part is a standard random coding bound. It is used in the CLT regime for a third-order analysis in [16] and a fourth-order analysis in [18]; it also comes up in the LD regime [20]. We set an arbitrary distribution $P_X \in \mathcal{P}$ to generate the i.i.d. random codebook and employ a maximum likelihood decoder. To bound the probability $\mathbb{P}[\iota(\mathbf{X}; \mathbf{Y}) \leq \tau]$, we replace the Edgeworth expansion in [18, eq. (5.30)], which gives the refined asymptotics of the Berry-Esseen theorem, with its moderate deviations version from [2, Ch. 8, Th. 2]. Note that the Edgeworth expansion yields an additive remainder term $O(1/n)$ to the normal term; this remainder becomes too large for the entire range of probabilities in (6). Therefore, a moderate deviation result that yields a multiplicative remainder term $(1 + o(1))$ is desired. We apply the large deviations result in [24, Th. 3.4] to bound the probability $\mathbb{P}[\iota(\bar{\mathbf{X}}; \mathbf{Y}) \geq \iota(\mathbf{X}; \mathbf{Y}) \geq \tau]$, where \mathbf{X} and $\bar{\mathbf{X}}$ denote the transmitted random codeword and an independent codeword drawn from the same distribution, respectively. This bound replaces the bounds in [18, eq. (7.25)-(7.27)] and refines the large deviations bound [3, Lemma 47] used in [16, Th. 53]. We show an achievability result as a function of $I(P_X)$, $V_u(P_X)$, and $\text{Sk}_u(P_X)$. If $P_X = P_X^* \in \mathcal{P}^*$, the resulting bound is (53) with $A_0(P_X^*)$ replaced by zero. We then optimize the bound over P_X using the second-, first- and zeroth-order Taylor series expansions around $P_X^* \in \mathcal{P}^*$ of $I(P_X)$, $V_u(P_X)$, and $\text{Sk}_u(P_X)$, respectively. Interestingly, the right-hand side of (53) is achieved using

$$P_X = P_X^* - \frac{Q^{-1}(\epsilon_n)}{2\sqrt{nV_{\epsilon_n}}} \tilde{\mathbf{J}} \mathbf{v}(P_X^*) \in \mathcal{P} \quad (55)$$

instead of a dispersion-achieving input distribution $P_X^* \in \mathcal{P}^*$ to generate i.i.d. random codewords. Note that despite being in the neighborhood of a dispersion-achieving P_X^* , P_X in (55), itself, might not belong to \mathcal{P}^* .

³There is a sign error in [18, eq. (3.1)-(3.2)], which then propagates through the rest of the paper. The sign of the terms with $S(P_X)$ should be positive rather than negative in both equations. The error in the achievability result originates in [18, eq. (7.15) and (7.19)], where it is missed that $\text{Sk}(-X) = -\text{Sk}(X)$ for any random variable X . The error in the converse result also stems from the sign error in [18, eq. (6.8)].

In the second-order MD result in [13], Altuğ and Wagner apply the non-asymptotic bound in [12, Cor. 2 on p. 140], which turns out to be insufficiently sharp for the derivation of the third-order term. See Section IV-C for the details of the proof. ■

We require the condition $V_{\epsilon_n} > 0$ in Theorem 1 since the moderate (Theorem 3 in Section IV-A) and large deviations results (Theorems 4 and 5 in Section IV-B) apply only to the random variables with positive variance. In the CLT regime, [3, Th. 45 and 48] and [17, Prop. 9-10] derive bounds on the non-Gaussianity for DMCs with $V_{\epsilon_n} = 0$. If $V_{\epsilon_n} = 0$, the scaling of the non-Gaussianity changes according to whether the DMC is exotic [3, p. 2331], which most DMCs do not satisfy, and whether ϵ_n is less than, equal to, or greater than $\frac{1}{2}$. A summary of the non-Gaussianity terms under these cases appears in [17, Fig. 1].

The condition $\mathcal{X}^\dagger = \mathcal{X}^*$ is a technical one that yields a closed-form solution (55) for the input distribution achieving the lower bound \underline{S} . If that condition is not satisfied, then the second term in (55) is replaced by the solution to the convex optimization problem (43), and $A_0(P_X^*)$ in (54) is replaced by the optimal value of (43).

Theorem 2: Under the conditions of Theorem 1,

$$\zeta(n, \epsilon_n) \leq \frac{1}{2} \log n + \overline{S} Q^{-1}(\epsilon_n)^2 + O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right) + O(1), \quad (56)$$

where

$$\overline{S} \triangleq \max_{P_X^* \in \mathcal{P}^*} \left(\frac{\text{Sk}_u(P_X^*) \sqrt{V_{\epsilon_n}}}{6} + \frac{1}{2} + A_0(P_X^*) - A_1(P_X^*) \right). \quad (57)$$

Proof: The proof of Theorem 2 combines the converse bound from [17, Prop. 6], which is derived from the meta-converse bound [3, Th. 27], and a saddlepoint result in [18, Lemma 14], which involves a maximization over an input distribution $P_X \in \mathcal{P}$ and a minimization over an output distribution $Q_Y \in \mathcal{Q}$. Combining these results and not deriving the $O(1)$ term in (56) yield a much simpler proof than that in [18]. While [18, proof of Th. 4] relies on the asymptotic expansion of the Neyman-Pearson Lemma (the $\beta_{1-\epsilon}(P, Q)$ function defined in [3, eq. (100)]), the use of [17, Prop. 6] allows us to bypass this part. After carefully choosing the parameter δ in [17, Prop. 6], the problem reduces to a single-letter minimax problem involving the quantities $D(P_{Y|X} \| Q_{Y|P_X})$ and $V(P_{Y|X} \| Q_{Y|P_X})$, where the maximization is over $P_X \in \mathcal{P}$ and the minimization is over $Q_Y \in \mathcal{Q}$. Then, similar to the steps in [18, eq. (8.22)], for the maximization over P_X , we separate the cases where $\|P_X - P_X^*\| \leq c_0 \frac{Q^{-1}(\epsilon_n)}{\sqrt{n}}$ or not, where $P_X^* \in \mathcal{P}^*$, and $c_0 > 0$ is a constant. Applying [18, Lemmas 14 and 9-iii] completes the proof. See Section IV-D for the details. ■

The constant terms \underline{S} and \overline{S} in [18] depend on whether the information density random variable $\iota(X; Y)$ is a lattice or non-lattice random variable because both the Edgeworth expansion and the large deviation result used in [18] take distinct forms for lattice and non-lattice random variables. The BSC is analyzed separately in [18, Th. 7] since the information

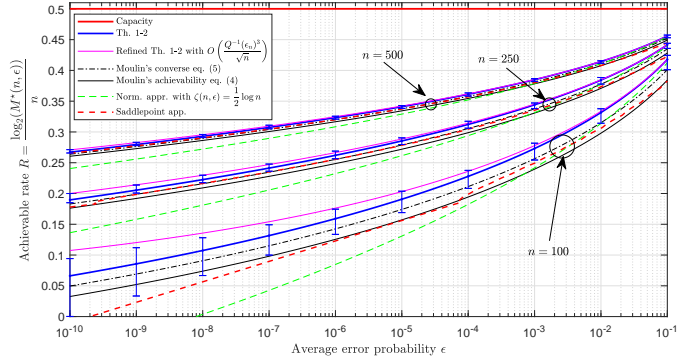


Fig. 1. The expansion from Theorems 1 and 2, excluding the $O(\cdot)$ terms, is shown for the BSC(0.11) with $\epsilon \in [10^{-10}, 10^{-1}]$ and $n = \{100, 250, 500\}$. The error bars correspond to the non-asymptotic achievability and converse bounds from [3, Th. 33 and 35]; the normal approximation, which achieves $\zeta(n, \epsilon) = \frac{1}{2} \log n$, is from [16, Th. 53]; Moulin's results are from [18, Th. 7]; the saddlepoint approximation is from [21, Th. 1] and [22, Sec. III-D].

density of the BSC is lattice. A single proof holds for lattice and non-lattice cases if we do not attempt to bound the $O(1)$ term as in this paper.

A. The tightness of Theorem 1 and Theorem 2

If the channel satisfies $|\mathcal{P}^*| = 1$, $A_0(P_X^*) = A_1(P_X^*) = 0$, and $\eta(P_X^*) = 0$, then achievability (53) and converse (56) bounds yield the channel skewness (9)

$$S = \frac{\text{Sk}_u(P_X^*) \sqrt{V_{\min}}}{6} + \frac{1}{2}. \quad (58)$$

Cover-Thomas symmetric channels [23, p. 190] satisfy all conditions;⁴ the BSC is an example. Further, if ϵ_n satisfies $Q^{-1}(\epsilon_n) = O(n^{1/6})$, then the $O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right)$ in (53) and (56) is dominated by the $O(1)$ term, giving that for Cover-Thomas symmetric channels, $\zeta(n, \epsilon_n) = \frac{1}{2} \log n + S Q^{-1}(\epsilon_n)^2 + O(1)$. For the BSC with crossover probability 0.11, Fig. 1 compares asymptotic expansions for the maximum achievable rate, $\frac{\log_2 M^*(n, \epsilon_n)}{n}$, dropping $o(\cdot)$ and $O(\cdot)$ terms except where noted otherwise. The curves plotted in Fig. 1 include Theorems 1 and 2 both with and without the leading term of $O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right)$ computed, various other asymptotic expansions in the CLT and LD regimes, and the non-asymptotic bounds from [3, Th. 33 and 35]. The leading term of $O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right)$ in Theorems 1 and 2 are computed in Theorems 7 and 8 in Section VI below. Among these asymptotic expansions, Theorems 1 and 2 ignoring the $O(\cdot)$ are the closest to the non-asymptotic bounds for most (n, ϵ) pairs shown, which highlights the significance of the channel skewness.

In [19], Altuğ and Wagner show that in the LD regime, for Gallager-symmetric channels, the prefactors in the lower and upper bounds on the error probability have the same order; that order depends on whether the channel is singular or nonsingular. Extending the analysis in [18, Sec. III-C-2]) to any Gallager-symmetric channel shows that Gallager-symmetric channels satisfy $A_0(P_X^*) = A_1(P_X^*) = 0$, but

⁴Channels that are (i) Cover-Thomas weakly symmetric, have (ii) $|\mathcal{X}| = |\mathcal{Y}|$ and (iii) a positive definite J satisfy the same conditions [18, Prop. 6].

$\eta(P_X^*)$ is not necessarily zero (see [18, Sec. III-C-2]) for a counterexample), which means that (53) and (56) are not tight up to the $O(1)$ term for some Gallager-symmetric channels. The findings in [19] suggest that Theorem 1 or Theorem 2 or both could be improved for some channels. The main difference between the achievability bounds in [19], [20] and ours is that [20] bounds the error probability by

$$\mathbb{P}[\mathcal{D}] + (M-1)\mathbb{P}[\mathcal{D}^c \cap \{i(\bar{\mathbf{X}}; \mathbf{Y}) \geq i(\mathbf{X}; \mathbf{Y})\}], \quad (59)$$

where

$$\mathcal{D} \triangleq \left\{ \log \frac{P_{Y|X}^n(\mathbf{Y}|\mathbf{X})}{Q_Y^n(\mathbf{Y})} < \tau \right\} \quad (60)$$

$$Q_Y(y) \triangleq c \left(\sum_{x \in \mathcal{X}} P_X(x) P_{Y|X}(y|x)^{1+\rho} \right)^{1+\rho}, \quad y \in \mathcal{Y}. \quad (61)$$

Here Q_Y is the tilted output distribution, and $\rho \in [0, 1]$, τ , and c are some constants. Our achievability bound uses a special case of (61) with $\rho = 0$, giving $Q_Y = P_Y$. Whether the more general bound in (61) yields an improved bound in the MD regime is a question for future work.

IV. PROOFS OF THEOREMS 1 AND 2

We begin by presenting the supporting lemmas used to bound the probability terms that appear in the proofs of Theorems 1 and 2.

A. Moderate deviations asymptotics

Theorem 3, stated next, is a moderate deviations result that bounds the probability that the sum of n i.i.d. random variables normalized by a factor $\frac{1}{\sqrt{n}}$ deviates from the mean by $o(\sqrt{n})$. The resulting probability is an MD sequence (6).

Theorem 3 (Petrov [2, Ch. 8, Th. 4]): Let X_1, \dots, X_n be independent random variables. Let $\mathbb{E}[X_i] = 0$ for $i = 1, \dots, n$, $\sigma^2 = \frac{1}{n} \sum_{i=1}^n \text{Var}[X_i] > 0$, $\mu_k = \frac{1}{n} \sum_{i=1}^n \mathbb{E}[X_i^k]$ for $k \geq 3$, and $\text{Sk} = \frac{\mu_3}{\sigma^3}$. Define

$$S_n \triangleq \frac{1}{\sqrt{n\sigma^2}} \sum_{i=1}^n X_i \quad (62)$$

$$F_n(x) \triangleq \mathbb{P}[S_n \leq x]. \quad (63)$$

Suppose that there exist some positive constants t_0 and H such that the moment generating function (MGF) satisfies

$$\mathbb{E}[\exp\{tX_i\}] < H \quad (64)$$

for all $|t| \leq t_0$ and $i = 1, \dots, n$. This condition is called Cramér's condition. Let $x > 1$ and $x = o(\sqrt{n})$. Then, it holds that

$$1 - F_n(x) = Q(x) \exp \left\{ \frac{x^3}{\sqrt{n}} \lambda_n \left(\frac{x}{\sqrt{n}} \right) \right\} \left(1 + O \left(\frac{x}{\sqrt{n}} \right) \right) \quad (65)$$

$$F_n(-x) = Q(x) \exp \left\{ \frac{-x^3}{\sqrt{n}} \lambda_n \left(\frac{-x}{\sqrt{n}} \right) \right\} \left(1 + O \left(\frac{x}{\sqrt{n}} \right) \right), \quad (66)$$

where

$$\lambda_n(x) \triangleq \sum_{i=0}^{\infty} a_i x^i \quad (67)$$

is Cramér's series whose first two coefficients are

$$a_0 = \frac{\text{Sk}}{6} \quad (68)$$

$$a_1 = \frac{(\mu_4 - 3\sigma^4)\sigma^2 - 3\mu_3^2}{24\sigma^6}. \quad (69)$$

The $O(\cdot)$ terms in (65)–(66) constitute a bottleneck in deriving the $O(1)$ terms in (53) and (56), that is, one needs to compute the leading term of the $O(\cdot)$ terms in (65)–(66) in order to compute the $O(1)$ terms in our achievability and converse bounds.

Inverting Theorem 3, namely, obtaining an expansion for x in terms y where $F_n(-x) = Q(y)$, is advantageous in many applications. Such an expansion gives the percentile value given a probability satisfying the MD sequence (6). In the CLT regime, i.e., $F_n(-x) \in (0, 1)$ is equal to a value independent of n , that expansion is known as the Cornish-Fisher theorem [29] that inverts the Edgeworth expansion. The following lemma is an extension of the Cornish-Fisher theorem to the MD regime.

Lemma 1: Let X_1, \dots, X_n satisfy the conditions in Theorem 3. Let $y \triangleq Q^{-1}(\epsilon_n) = o(\sqrt{n})$. Suppose that $F_n(-x) = Q(y) = \epsilon_n$, then

$$x = y - \frac{b_0 y^2}{\sqrt{n}} + \frac{b_1 y^3}{n} + O \left(\frac{y^4}{n^{3/2}} \right) + O \left(\frac{1}{\sqrt{n}} \right), \quad (70)$$

where

$$b_0 \triangleq \frac{\text{Sk}}{6} \quad (71)$$

$$b_1 \triangleq \frac{3(\mu_4 - 3\sigma^4)\sigma^2 - 4\mu_3^2}{72\sigma^6}. \quad (72)$$

Proof: See Appendix A. ■

A weaker version of Lemma 1 with only the first two terms in (70), and with ϵ_n decaying polynomially with n is proved in [30, Lemma 7]. We use Theorem 3 and Lemma 1 to bound the probability $\mathbb{P}[i(\mathbf{X}; \mathbf{Y}) \leq \tau]$, where τ is a threshold satisfying the condition in Theorem 3, and the resulting probability is an MD sequence (6).

B. Strong large deviations asymptotics

Theorem 4, below, is a strong large deviations result for an arbitrary sequence of random vectors in \mathbb{R}^d .

Let $\{\mathbf{S}_n\}_{n=1}^{\infty}$ be a sequence of d -dimensional random vectors. Denote the MGF of the random vector \mathbf{S}_n by

$$\phi_n(\mathbf{z}) = \mathbb{E}[\exp\{\langle \mathbf{z}, \mathbf{S}_n \rangle\}] \quad (73)$$

for $\mathbf{z} \in \mathbb{C}^d$, and the normalized cumulant generating function of \mathbf{S}_n by

$$\kappa_n(\mathbf{z}) = \frac{1}{n} \log \phi_n(\mathbf{z}). \quad (74)$$

The Fenchel-Legendre transform of κ_n is given by

$$\Lambda_n(\mathbf{x}) = \sup_{\mathbf{t} \in \mathbb{R}^d} \{\langle \mathbf{t}, \mathbf{x} \rangle - \kappa_n(\mathbf{t})\}, \quad (75)$$

where $\mathbf{x} \in \mathbb{R}^d$ and $\langle \mathbf{t}, \mathbf{x} \rangle \triangleq \sum_{i=1}^d t_i x_i$. The quantity (75) is commonly known as the *rate function* in the large deviations literature [31, Ch. 2.2].

Theorem 4 (Chaganty and Sethuraman [24, Th. 3.4]): Let $\mathbf{S}_n = (S_{n,1}, \dots, S_{n,d})$, $n = 1, 2, \dots$ be a sequence of d -dimensional random vectors, and $\{\mathbf{a}_n\}_{n=1}^\infty$ be a bounded sequence of d -dimensional vectors. Assume that

- (S) κ_n is bounded below and above, and is analytic in \mathcal{D}^d , where $\mathcal{D} \triangleq \{z \in \mathbb{C}: |z| < c\}$ and c is a finite constant;
 (ND) there exists a sequence $\{s_n\}_{n=1}^\infty$ and constants c_0 and c_1 that satisfy

$$\nabla \kappa_n(\mathbf{s}_n) = \mathbf{a}_n \quad (76)$$

$$0 < c_0 < s_{n,j} < c_1 < c \text{ for all } j \in [d] \text{ and } n \geq 1, \quad (77)$$

where c is the constant given in condition (S), and that the Hessian matrix $\nabla^2 \kappa_n(\mathbf{s}_n)$, which is a covariance matrix of a tilted distribution obtained from \mathbf{S}_n , is positive definite with a minimum eigenvalue bounded away from zero for all n ;

- (NL) there exists $\delta_0 > 0$ such that

$$\sup_{\mathbf{t}: \delta_1 < \|\mathbf{t}\| \leq \delta_2} \left| \frac{\phi_n(\mathbf{s}_n + \mathbf{it})}{\phi_n(\mathbf{s}_n)} \right| = o(n^{-d/2}) \quad (78)$$

for any given δ_1 and δ_2 such that $0 < \delta_1 < \delta_0 < \delta_2$, where $i = \sqrt{-1}$ is the imaginary unit.

Then,

$$\mathbb{P}[\mathbf{S}_n \geq n\mathbf{a}_n] = \frac{C_{nl}}{n^{d/2}} \exp\{-n\Lambda_n(\mathbf{a}_n)\}(1 + o(1)), \quad (79)$$

where

$$C_{nl} \triangleq \frac{1}{(2\pi)^{d/2} \left(\prod_{j=1}^d s_{n,j} \right) \sqrt{\det(\nabla^2 \kappa_n(\mathbf{s}_n))}}. \quad (80)$$

Condition (S) of Theorem 4 is a *smoothness* assumption for the MGF κ_n , which is a generalization of Cramér's condition that appears in the large deviations theorem for the sum of i.i.d. random vectors [31, Th. 2.2.30]. Condition (S) implies that all moments of the tilted distribution obtained from \mathbf{S}_n are finite. Condition (ND) is used to satisfy that \mathbf{S}_n is a *non-degenerate* random vector, meaning that it does not converge in distribution to a random vector with $\ell < d$ dimensions, and that the rate function $\Lambda_n(\mathbf{a}_n)$ is bounded and does not decay to zero. The latter follows from the boundedness condition in (77), and implies that the probability of interest is in the LD regime. The left-hand side of (78) is a characteristic function of a tilted distribution obtained from the distribution of \mathbf{S}_n [24]; hence the supremum in (78) is strictly below 1 for any non-lattice random vector.⁵ Condition (NL) is used to guarantee that the absolute value of that characteristic function decays to zero fast enough outside a neighborhood of the origin, which makes the random vector \mathbf{S}_n behave like a sum of n non-lattice random vectors.

We apply Theorem 4 to the sequence of 2-dimensional non-lattice random vectors $(\iota(\mathbf{X}; \mathbf{Y}), \iota(\overline{\mathbf{X}}; \mathbf{Y}) - \iota(\mathbf{X}; \mathbf{Y}))$ to

⁵Characteristic function of a lattice random variable is periodic; and therefore, its absolute value takes 1 at a non-zero value.

bound the probability $\mathbb{P}[\iota(\overline{\mathbf{X}}; \mathbf{Y}) \geq \iota(\mathbf{X}; \mathbf{Y}) \geq \tau_n]$ for some sequence τ_n . Here, $\overline{\mathbf{X}}$ is a random codeword, that is independent of both \mathbf{X} and \mathbf{Y} .

When applied to the sum of n i.i.d. random variables $\mathbf{S}_n = \sum_{i=1}^n \mathbf{X}_i$, κ_n in (74) reduces to

$$\kappa(\mathbf{z}) = \log \mathbb{E}[\exp\{\langle \mathbf{z}, \mathbf{X}_1 \rangle\}]. \quad (81)$$

If \mathbf{X}_1 has a finite support, the expectation in (81) is bounded, and all moments of \mathbf{X}_1 are finite; therefore, condition (S) of Theorem 4 is satisfied. Further, the characteristic function of the sum of n i.i.d. random vectors is equal to n -th power of the characteristic function of one of the summands. Therefore, the left-hand side of (78) decays to zero exponentially fast for the sum of i.i.d. non-lattice random vectors, satisfying condition (NL) of Theorem 4 with room to spare.

We use the following strong large deviations result to bound the probability $\mathbb{P}[\iota(\overline{\mathbf{X}}; \mathbf{Y}) \geq \iota(\mathbf{X}; \mathbf{Y}) \geq \tau_n]$ with lattice $\iota(\mathbf{X}; \mathbf{Y})$ and $\iota(\overline{\mathbf{X}}; \mathbf{Y})$.

Theorem 5: Let $\{\mathbf{S}_n\}_{n=1}^\infty$ be a sequence of random vectors on \mathbb{R}^d . Suppose that $\mathbf{S}_n = (S_{n,1}, \dots, S_{n,d})$, and $S_{n,j}$ is a lattice random variable with a span $h_{n,j}$, i.e., $\mathbb{P}[S_{n,j} \in \{b_{n,j} + kh_{n,j}: k \in \mathbb{Z}\}] = 1$ for some $b_{n,j}$, such that there exist positive constants \underline{h}_j and \overline{h}_j satisfying $\underline{h}_j < h_{n,j} < \overline{h}_j$ for all $j \in [d]$, $n \geq 1$. Assume that conditions (S) and (ND) in Theorem 4 hold, and replace condition (NL) by

- (L) there exists $\lambda > 0$ such that for any given δ satisfying $0 < \delta < \lambda$,

$$\sup_{\mathbf{t}: \delta_j < |t_j| \leq \frac{\pi}{h_{n,j}} \text{ for } j \in [d]} \left| \frac{\phi_n(\mathbf{s}_n + \mathbf{it})}{\phi_n(\mathbf{s}_n)} \right| = o(n^{-d/2}). \quad (82)$$

Assume that $n\mathbf{a}_n$ is in the range of the random vector \mathbf{S}_n . Then,

$$\mathbb{P}[\mathbf{S}_n \geq n\mathbf{a}_n] = \frac{C_1}{n^{d/2}} \exp\{-n\Lambda_n(\mathbf{a}_n)\}(1 + o(1)), \quad (83)$$

where

$$C_1 \triangleq \frac{1}{(2\pi)^{d/2} \sqrt{\det(\nabla^2 \kappa_n(\mathbf{s}_n))}} \left(\prod_{j=1}^d \frac{h_{n,j}}{1 - \exp\{-s_{n,j} h_{n,j}\}} \right). \quad (84)$$

Proof: The one-dimensional lattice case, i.e., $d = 1$, is proved in [32, Th. 3.5]. The proof of the d -dimensional lattice case follows by inspecting the proofs for the d -dimensional non-lattice random vectors in [24, Th. 3.4] and the one-dimensional lattice random variables in [32, Th. 3.5]. Specifically, in the proof of [24, Th. 3.4], we replace [24, Th. 2.4] by [32, Th. 2.10]. The auxiliary result [32, Th. 2.10] gives the asymptotics of an expectation of a lattice random variable. The modification in the proof yields Theorem 5. ■

In the application of Theorem 5, if $\mathbf{S}_n = (S_{n,1}, \dots, S_{n,d})$ is a sum of n i.i.d. random vectors, where

$$S_{n,j} = \sum_{i=1}^n X_{i,j}, \quad j \in [d], \quad (85)$$

and $X_{1,j}$ is lattice distributed with a span h_j for $j \in [d]$, then

$$\sup_{\delta_j < |t_j| \leq \frac{\pi}{h_j}} \left| \frac{\phi^{(j)}(s_j + it_j)}{\phi^{(j)}(s_j)} \right| < 1, \quad j \in [d], \quad (86)$$

where $\phi^{(j)}(\cdot)$ is the MGF of $X_{1,j}$. The quantity $\frac{\phi^{(j)}(s_j + it_j)}{\phi^{(j)}(s_j)}$ is a characteristic function of a random variable with a span h_j ; therefore, it is a periodic function of t_j with a period of $\frac{2\pi}{h_j}$.⁶ The condition in (82) modifies the condition in (78) for lattice random vectors by considering a single period of that characteristic function. From (86) and the fact that \mathbf{S}_n is an i.i.d. sum, the left-hand side of (82) decays exponentially with n , and condition (L) is satisfied. Note that when $h_{n,j} \rightarrow 0$ for all (n, j) pairs, then \mathbf{S}_n converges to a non-lattice random vector, and the prefactor C_1 converges to the prefactor for the non-lattice random vectors, C_{nl} .

Altuğ and Wagner derive a large deviations bound in [20, Lemma 3] that applies to the sum of n i.i.d. 2-dimensional random vectors, where each summand can be either non-lattice or lattice. However, their prefactor is worse than both C_{nl} and C_1 . Since our achievability proof in Section IV-C relies on only the fact that the prefactor in the large deviation bound is a bounded constant (see (111), below), [20, Lemma 3] is also applicable in our achievability proof. If one seeks to derive the $O(1)$ term in (53), the tightness of the prefactor used in the probability bound would be important. Our converse proof in Section IV-D does not use the strong large deviations theorems presented in the current section.

If ϵ_n is constant, Theorem 1 follows from [16, Th. 53] and Theorem 2 follows from [17, Th. 1]. Therefore, we only consider the cases where the sequence $\{\epsilon_n\}_{n=1}^\infty$ satisfies the MD condition (6), and $\epsilon_n \rightarrow 0$ or $\epsilon_n \rightarrow 1$. Below, we prove the results for such sequences.

C. Proof of Theorem 1

The proof consists of two parts, and follows similar steps as in the achievability proof in [18]. First, we derive an achievability bound for an arbitrary input distribution $P_X \in \mathcal{P}$. Then, we optimize that achievability bound over all $P_X \in \mathcal{P}$.

Lemma 2: Suppose that ϵ_n satisfies (6). Fix some $P_X \in \mathcal{P}$ such that $(P_X, P_{Y|X})$ is a nonsingular pair and $V_u(P_X) > 0$ for all n . It holds that

$$\begin{aligned} & \log M^*(n, \epsilon_n) \\ & \geq nI(P_X) - \sqrt{nV_u(P_X)}Q^{-1}(\epsilon_n) + \frac{1}{2} \log n \\ & \quad + Q^{-1}(\epsilon_n)^2 \left(\frac{\text{Sk}_u(P_X)\sqrt{V_u(P_X)}}{6} + \frac{1 - \eta(P_X)}{2(1 + \eta(P_X))} \right) \\ & \quad + O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right) + O(1). \end{aligned} \quad (87)$$

We require $V_u(P_X) > 0$ in order to apply Theorems 3–5.

Proof of Lemma 2: We employ a random encoder. The codewords $\mathbf{f}(m) = (f_1(m), \dots, f_n(m))$, $m = 1, \dots, M$, are generated i.i.d. from the product distribution P_X^n . Let W be the sent message that is uniformly distributed on $[M]$, giving the joint distribution

$$\begin{aligned} & P_{W, \mathbf{f}(1), \dots, \mathbf{f}(M), \mathbf{Y}}(w, \mathbf{x}_1, \dots, \mathbf{x}_M, \mathbf{y}) \\ & = \frac{1}{M} \left(\prod_{m=1}^M P_X^n(\mathbf{x}_m) \right) P_{Y|X}^n(\mathbf{y}|\mathbf{x}_w). \end{aligned} \quad (88)$$

⁶Note that the argument of the supremum in (86) is equal to 1 at a non-zero value, making the left-hand side of (78) equal to 1.

Note that the triple $(\mathbf{f}(W), \mathbf{f}(m), \mathbf{Y})$, $m \neq W$, is distributed identically to $(\mathbf{X}, \bar{\mathbf{X}}, \mathbf{Y})$, where $P_{\mathbf{X}, \bar{\mathbf{X}}, \mathbf{Y}}(\mathbf{x}, \bar{\mathbf{x}}, \mathbf{y}) = P_X^n(\mathbf{x}^n)P_X^n(\bar{\mathbf{x}}^n)P_{Y|X}^n(\mathbf{y}|\mathbf{x})$. Define the random variables

$$Z \triangleq \iota(\mathbf{X}; \mathbf{Y}) \quad (89)$$

$$\bar{Z} \triangleq \iota(\bar{\mathbf{X}}; \mathbf{Y}). \quad (90)$$

The random variable \bar{Z} corresponds to the information density obtained from a sample from the random codebook, independent from both \mathbf{X} and the received vector \mathbf{Y} .

We define the information density random variables

$$Z(m) \triangleq \iota(\mathbf{f}(m); \mathbf{Y}) \quad (91)$$

$$= \sum_{i=1}^n \iota(f_i(m); Y_i) \quad (92)$$

$$= \sum_{i=1}^n \log \frac{P_{Y|X}(Y_i|f_i(m))}{P_Y(Y_i)}. \quad (93)$$

We use the maximum likelihood decoder, i.e., upon receiving the output symbols $\mathbf{Y} = \mathbf{y}$, the decoder outputs the message

$$\hat{W} = \arg \max_{m \in [M]} Z(m); \quad (94)$$

ties are broken uniformly at random.

1) *Error analysis:* Fix a threshold value τ_n

$$\tau_n = nI(P_X) - \sqrt{nV_u(P_X)}t_n, \quad (95)$$

where t_n will be specified in (103) below. Define the event

$$\mathcal{D} \triangleq \{Z(1) < \tau_n | W = 1\}. \quad (96)$$

The average error probability of the random code constructed above is bounded by

$$\begin{aligned} & \mathbb{P}[\hat{W} \neq W] \\ & \leq \mathbb{P}\left[\bigcup_{m \neq 1} \{Z(m) \geq Z(1) | W = 1\}\right] \end{aligned} \quad (97)$$

$$\leq \mathbb{P}[\mathcal{D}] + \mathbb{P}\left[\mathcal{D}^c \cap \bigcup_{m \neq 1} \{Z(m) \geq Z(1)\} | W = 1\right] \quad (98)$$

$$\leq \mathbb{P}[\mathcal{D}] + (M-1)\mathbb{P}[\bar{Z} \geq Z \geq \tau_n], \quad (99)$$

where the inequality (97) follows from the maximum likelihood decoder and the i.i.d. random code ensemble. Inequality (99) follows by applying the union bound to the second probability term in (98) and is a weakening of the random coding union (RCU) bound [3, Th. 16]. In the application of the RCU bound in [16, eq. (3.324)] where ϵ_n is a constant, the RCU bound is also bounded as in (99).

Define the sequences

$$h_n \triangleq \frac{1}{\sqrt{nV_u(P_X)}} \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{Q^{-1}(\epsilon_n)^2}{2}\right\} \quad (100)$$

$$= \frac{\min\{\epsilon_n, 1 - \epsilon_n\}Q^{-1}(\min\{\epsilon_n, 1 - \epsilon_n\})}{\sqrt{nV_u(P_X)}}(1 + o(1)) \quad (101)$$

$$\tilde{\epsilon}_n \triangleq \epsilon_n - h_n, \quad (102)$$

where (101) follows from [30, eq. (16)]. Here, h_n is chosen so that $\log M$ is maximized up to the $O(Q^{-1}(\epsilon_n)^2)$ term given that the right-hand side of (99) is bounded by ϵ_n .

We set t_n in (96) as

$$\mathbb{P}[\mathcal{D}] = \mathbb{P}\left[\frac{Z - nI(P_X)}{\sqrt{nV_u(P_X)}} \leq -t_n\right] = \tilde{\epsilon}_n. \quad (103)$$

Since the channel is a DMC, the random variable $\iota(X; Y)$ has a finite support and is bounded. Therefore, Cramér's condition in Theorem 3 is satisfied. Applying the MD result in Lemma 1 to (103), we get

$$t_n = Q^{-1}(\tilde{\epsilon}_n) - \frac{\text{Sk}_u(P_X)Q^{-1}(\tilde{\epsilon}_n)^2}{6\sqrt{n}} + O\left(\frac{Q^{-1}(\tilde{\epsilon}_n)^3}{n}\right) + O\left(\frac{1}{\sqrt{n}}\right). \quad (104)$$

We compute the first two derivatives of the $Q^{-1}(x)$ function as

$$(Q^{-1})'(x) = \frac{1}{Q'(Q^{-1}(x))} = \frac{-1}{g(x)} \quad (105)$$

$$(Q^{-1})''(x) = -\frac{Q^{-1}(x)}{g(x)^2}, \quad (106)$$

where $g(x) \triangleq \frac{1}{\sqrt{2\pi}} \exp\{-Q^{-1}(x)^2/2\}$. As $x \rightarrow 0^+$, it holds that [30, eq. (15)-(16)]

$$g(x) = xQ^{-1}(x)(1 + o(1)). \quad (107)$$

By taking the Taylor series expansion of $Q^{-1}(\cdot)$ around ϵ_n and using (104)–(107), we get⁷

$$t_n = Q^{-1}(\epsilon_n) - \frac{\text{Sk}_u(P_X)Q^{-1}(\epsilon_n)^2}{6\sqrt{n}} + O\left(\frac{Q^{-1}(\epsilon_n)^3}{n}\right) + O\left(\frac{1}{\sqrt{n}}\right). \quad (108)$$

Next, we bound the probability $\mathbb{P}[\bar{Z} \geq Z \geq \tau_n]$. Define the random vector $\mathbf{U} \triangleq (U_1, U_2) = (Z, \bar{Z} - Z)$, and the sequence

$$\mathbf{a}_n = (a_{n,1}, a_{n,2}) = \left(\frac{\tau_n}{n}, 0\right). \quad (109)$$

Applying Theorem 4 or Theorem 5 depending on whether $\iota(X; Y)$ is non-lattice or lattice, we get

$$\mathbb{P}[\bar{Z} \geq Z \geq \tau_n] = \mathbb{P}[\mathbf{U} \geq n\mathbf{a}_n] \quad (110)$$

$$\leq \frac{C}{n} \exp\{-n\Lambda(\mathbf{a}_n)\}(1 + o(1)), \quad (111)$$

where

$$C = \begin{cases} C_{\text{nl}} & \text{if } \iota(X; Y) \text{ is non-lattice} \\ C_1 & \text{otherwise.} \end{cases} \quad (112)$$

$$\Lambda(\mathbf{a}_n) = \sup_{\mathbf{s}_n \in \mathbb{R}^2} \{\langle \mathbf{a}_n, \mathbf{s}_n \rangle - \kappa(\mathbf{s}_n)\} \quad (113)$$

$$\kappa(\mathbf{s}_n) = \frac{1}{n} \log \mathbb{E}[\exp\{\langle \mathbf{s}_n, \mathbf{U} \rangle\}]. \quad (114)$$

⁷The derivation of the asymptotics (108) is the only step where the analysis differs depending on whether $\epsilon_n \rightarrow 0$ or $\epsilon_n \rightarrow 1$. If $\epsilon_n \rightarrow 1$, we use (104)–(107) after the step $Q^{-1}(\epsilon_n) = -Q^{-1}(1 - \epsilon_n)$.

Note that the functions $\kappa(\cdot)$ and $\Lambda(\cdot)$ do not depend on n since \mathbf{U} is an i.i.d. sum. The rate function $\Lambda(\mathbf{a}_n)$ has the Taylor series expansion

$$\Lambda(\mathbf{a}_n) = I(P_X) + (a_{n,1} - I(P_X)) + \frac{(a_{n,1} - I(P_X))^2}{(1 + \eta(P_X))V_u(P_X)} + O(|a_{n,1} - I(P_X)|^3) \quad (115)$$

$$= a_{n,1} + \frac{1}{n} \frac{Q^{-1}(\epsilon_n)^2}{1 + \eta(P_X)} + O\left(\frac{Q^{-1}(\epsilon_n)^3}{n^{3/2}}\right) + O\left(\frac{1}{n}\right). \quad (116)$$

In the application of Theorems 4 and 5, conditions (S), (NL), and (L) are already satisfied since U_1 and U_2 have finite supports. The verification of condition (ND) and the derivation of (116) appear in Appendix B.

We set

$$\begin{aligned} \log M &= nI(P_X) - \sqrt{nV_u(P_X)}Q^{-1}(\epsilon_n) + \frac{1}{2} \log n \\ &+ Q^{-1}(\epsilon_n)^2 \left(\frac{\text{Sk}_u(P_X)\sqrt{V_u(P_X)}}{6} + \frac{1 - \eta(P_X)}{2(1 + \eta(P_X))} \right) \\ &+ O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right) + O(1). \end{aligned} \quad (117)$$

From (95), (108), (109), (111), and (116), we get

$$M\mathbb{P}[\bar{Z} \geq Z \geq \tau_n] \leq h_n, \quad (118)$$

where h_n is defined in (100). Combining (102), (103), and (118) completes the proof. \blacksquare

To complete the proof of Theorem 1, it only remains to maximize the right-hand side of (87) over $P_X \in \mathcal{P}$. The following arguments extend the proof of [18, Lemma 9] to the MD regime. Define

$$G(P_X) \triangleq -\sqrt{V_u(P_X)}Q^{-1}(\epsilon_n). \quad (119)$$

Let \mathbf{g} be a vector whose components approach zero with a rate $O\left(\frac{Q^{-1}(\epsilon_n)}{\sqrt{n}}\right)$ satisfying $\mathbf{g}^\top \mathbf{1} = 0$, and $f(\mathbf{g})$ be the right-hand side of (87) evaluated at $P_X = P_X^* + \mathbf{g} \in \mathcal{P}$ for some $P_X^* \in \mathcal{P}^*$. We apply the Taylor series expansion to $f(\mathbf{g})$ and get

$$\begin{aligned} f(\mathbf{g}) &\triangleq nI(P_X^*) + n\mathbf{g}^\top \nabla I(P_X^*) + \frac{n}{2} \mathbf{g}^\top \nabla^2 I(P_X^*) \mathbf{g} \\ &+ O(n\|\mathbf{g}\|^3) + \sqrt{n}G(P_X^*) + \sqrt{n}\mathbf{g}^\top \nabla G(P_X^*) \\ &+ \sqrt{n}O(\|\mathbf{g}\|^2) + \frac{1}{2} \log n \\ &+ Q^{-1}(\epsilon_n)^2 \left(\frac{\text{Sk}_u(P_X^*)\sqrt{V_u(P_X^*)}}{6} + \frac{1 - \eta(P_X^*)}{2(1 + \eta(P_X^*))} \right) \\ &+ O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right) + O(1) \end{aligned} \quad (120)$$

$$\begin{aligned} &= n\mathbf{g}^\top \nabla I(P_X^*) + \frac{n}{2} \mathbf{g}^\top \nabla^2 I(P_X^*) \mathbf{g} \\ &+ \sqrt{n}\mathbf{g}^\top \nabla G(P_X^*) + b, \end{aligned} \quad (121)$$

where b is the right-hand side of (87), which is independent of \mathbf{g} . From (39) and [12, Th. 4.5.1], for every \mathbf{g} such that $P_X^* + \mathbf{g}$ is a valid probability distribution and n large enough, we have

$$f(\mathbf{g}) \leq \sup_{\mathbf{g}' \in \mathcal{L}} \left\{ -\frac{n}{2} \mathbf{g}'^\top \mathbf{J} \mathbf{g}' + \sqrt{n}\mathbf{g}'^\top \nabla G(P_X^*) + b \right\}, \quad (122)$$

where \mathbf{J} and \mathcal{L} are defined in (41)–(42); and the right-hand side of (122) is achieved by some \mathbf{g} with $g_x = 0$ for $x \notin \mathcal{X}^\dagger$. Since P_X^* is dispersion-achieving, $\mathbf{g}^\top \nabla G(P_X^*) = 0$ for any \mathbf{g} in the kernel of \mathbf{J} . Therefore, the problem (122) reduces to

$$\sup_{\mathbf{g} \in \mathcal{L}} \mathbf{g}^\top \mathbf{h} - \frac{1}{2} \mathbf{g}^\top \mathbf{J} \mathbf{g}, \quad (123)$$

where \mathbf{h} is the orthogonal projection of $\frac{\nabla G(P_X^*)}{\sqrt{n}}$ onto the row space of \mathbf{J} . Under the assumption $\mathcal{X}^\dagger = \mathcal{X}^*$, the supremum in (123) is achieved by

$$\mathbf{g}^* = \tilde{\mathbf{J}} \mathbf{h}, \quad (124)$$

where $\tilde{\mathbf{J}}$ is given in (45), and the value of supremum in (123) is $A_0(P_X^*)Q^{-1}(\epsilon_n)^2$. See Appendix C for the details. Combining the values of b and the value of (123) gives the maximum of (87) over all input distributions $P_X \in \mathcal{P}$ and completes the proof of Theorem 1.

D. Proof of Theorem 2

The proof analyzes the converse bound in [17, Prop. 6] using the techniques in [18, Lemmas 9 and 14]. We first introduce the binary hypothesis tests, which are fundamental in most converse theorems in the literature.

Let P and Q be two distributions on a common alphabet \mathcal{X} . Consider the binary hypothesis test

$$H_0: X \sim P \quad (125)$$

$$H_1: X \sim Q. \quad (126)$$

A randomized test between those two distributions is defined by a probability transition kernel $P_{W|X}: \mathcal{X} \rightarrow \{0, 1\}$, where 0 indicates that the test chooses H_0 , i.e., P , and 1 indicates that the test chooses H_1 , i.e., Q . We define the minimum achievable type-II error if the type-I error is bounded by $1 - \alpha$ as [3, eq. (100)]

$$\beta_\alpha(P, Q) = \min_{\delta: \sum_{x \in \mathcal{X}} P(x)P_{W|X}(0|x) \geq \alpha} \sum_{x \in \mathcal{X}} Q(x)P_{W|X}(0|x). \quad (127)$$

See Section V for the tight asymptotics of $\beta_\alpha(P, Q)$ in the MD regime.

Next, we define the divergence spectrum [33, Ch. 4], [17], which gives a lower bound on $\beta_{1-\epsilon}(P, Q)$ (see (131), below)

$$D_s^\epsilon(P||Q) \triangleq \sup \left\{ \gamma \in \mathbb{R}: \mathbb{P} \left[\log \frac{P(X)}{Q(X)} \leq \gamma \right] \leq \epsilon \right\}, \quad (128)$$

where $\epsilon \in (0, 1)$, $P, Q \in \mathcal{P}$, and $X \sim P$.

Lemma 3 ([17, Prop. 6]): Let $\epsilon_n \in (0, 1)$ and $P_{Y|X}$ be a DMC. Then, for any $\delta_n \in (0, 1 - \epsilon_n)$, we have

$$\log M^*(n, \epsilon_n) \leq \min_{Q_Y^{(n)} \in \mathcal{Q}^n} \max_{\mathbf{x} \in \mathcal{X}^n} D_s^{\epsilon_n + \delta_n}(P_{Y|\mathbf{X}=\mathbf{x}}||Q_Y^{(n)}) - \log \delta_n, \quad (129)$$

where $P_{Y|\mathbf{X}=\mathbf{x}} = \prod_{i=1}^n P_{Y|X=x_i}$.

Polyanskiy *et al.*'s meta-converse bound in [3, Th. 27] states that

$$\log M \leq -\log \beta_{1-\epsilon_n}(\hat{P}_{\mathbf{X}} \times P_{Y|X}^n, \hat{P}_{\mathbf{X}} \times Q_Y^{(n)}) \quad (130)$$

for any $Q_Y^{(n)} \in \mathcal{Q}^n$, where $\hat{P}_{\mathbf{X}} \in \mathcal{P}^n$ is the codeword distribution induced by the encoder, and then takes the minimum over $Q_Y^{(n)} \in \mathcal{Q}^n$ and maximum over $P_X^{(n)} \in \mathcal{P}^n$ to obtain a code-independent bound. Lemma 3 relaxes the meta-converse bound by bounding the right-hand side of (130) as

$$-\log \beta_{1-\epsilon_n}(\hat{P}_{\mathbf{X}} \times P_{Y|X}^n, \hat{P}_{\mathbf{X}} \times Q_Y^{(n)}) \leq D_s^{\epsilon_n + \delta_n}(\hat{P}_{\mathbf{X}} \times P_{Y|X}^n || \hat{P}_{\mathbf{X}} \times Q_Y^{(n)}) - \log \delta_n \quad (131)$$

$$\leq \max_{\mathbf{x} \in \mathcal{X}^n} D_s^{\epsilon_n + \delta_n}(P_{Y|\mathbf{X}=\mathbf{x}} || Q_Y^{(n)}) - \log \delta_n \quad (132)$$

for any $1 - \epsilon_n > \delta_n > 0$, where (131) follows from [3, eq. (100)], and (132) follows from [17, Lemma 4]. The advantage of Lemma 3 over the meta-converse bound is that the optimization problem in Lemma 3 can be converted into a simpler single-letter minimax problem by analyzing the asymptotics of the $D_s^{\epsilon_n}(P_{Y|\mathbf{X}=\mathbf{x}} || Q_Y^{(n)})$ function (see Lemma 4 below). A similar simplification to a single-letter problem for the converse results using the β_α function is possible (i) under the average error probability criterion for channels that satisfy certain symmetry conditions [3, Th. 28] (e.g., Cover-Thomas symmetric channels satisfy these symmetry conditions) and (ii) under the maximal error probability criterion for arbitrary DMCs [3, Th. 31]. Theorem 8, below, refines Theorem 2 for Cover-Thomas symmetric channels by applying [3, Th. 28]. The disadvantage of using Lemma 3 is that in general, it is not tight enough to obtain the tightest $O(\cdot)$ terms in (56).

Lemma 4, below, derives the asymptotics of $D_s^{\epsilon_n}(P_{Y|\mathbf{X}=\mathbf{x}} || Q_Y^{(n)})$ in the MD regime when $Q_Y^{(n)} = Q_Y^n$ is an i.i.d. distribution.

Lemma 4: Fix some $\mathbf{x} \in \mathcal{X}^n$ and $Q_Y \in \mathcal{Q}$. Assume that $\{\epsilon_n\}_{n=1}^\infty$ is an MD sequence (6). It holds that

$$\begin{aligned} D_s^{\epsilon_n}(P_{Y|\mathbf{X}=\mathbf{x}} || Q_Y^n) &= nD_{\mathbf{x}} - \sqrt{nV_{\mathbf{x}}}Q^{-1}(\epsilon_n) + \frac{S_{\mathbf{x}}\sqrt{V_{\mathbf{x}}}}{6}Q^{-1}(\epsilon_n)^2 \\ &\quad + O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right) + O(1), \end{aligned} \quad (133)$$

where

$$D_{\mathbf{x}} \triangleq D(P_{Y|X} || Q_Y | \hat{P}_{\mathbf{x}}) \quad (134)$$

$$V_{\mathbf{x}} \triangleq V(P_{Y|X} || Q_Y | \hat{P}_{\mathbf{x}}) \quad (135)$$

$$S_{\mathbf{x}} \triangleq \frac{T(P_{Y|X} || Q_Y | \hat{P}_{\mathbf{x}})}{V(P_{Y|X} || Q_Y | \hat{P}_{\mathbf{x}})^{3/2}}. \quad (136)$$

Proof: See Appendix D. ■

By the inequality (131), divergence spectrum gives an upper bound on $-\log \beta_{1-\epsilon_n}$. Further, inspecting (133) and the asymptotics of the $\beta_{1-\epsilon_n}$ function in (162) below, we see that setting $\log \delta_n = -\frac{Q^{-1}(\epsilon_n)^2}{2} - \frac{1}{2} \log n$ in (129) yields a tight upper bound up to the $O(\cdot)$ terms in (133).

To find the minimax of $D_s^{\epsilon_n}(P_{Y|\mathbf{X}=\mathbf{x}} || Q_Y^n)$ in (133), we define the asymptotic expansion $\xi: \mathcal{P} \times \mathcal{P} \rightarrow \mathbb{R}$ in (137) at the top of the next page, where $P_Y^{(o)} = P_X^{(o)} P_{Y|X}$ is the output distribution induced by $P_X^{(o)}$.

$$\begin{aligned} \xi(P_X^{(i)}, P_X^{(o)}) &\triangleq nD(P_{Y|X} \| P_Y^{(o)} | P_X^{(i)}) - \sqrt{nV(P_{Y|X} \| P_Y^{(o)} | P_X^{(i)})} Q^{-1}(\epsilon_n) \\ &+ \frac{\text{Sk}(P_{Y|X} \| P_Y^{(o)} | P_X^{(i)}) \sqrt{V(P_{Y|X} \| P_Y^{(o)} | P_X^{(i)})}}{6} Q^{-1}(\epsilon_n)^2 + O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right) + O(1) \end{aligned} \quad (137)$$

The minimax of the first term $nD(P_{Y|X} \| P_Y^{(o)} | P_X^{(i)})$ in (137) satisfies the saddlepoint property (e.g., [34, Cor. 4.2])

$$D(P_{Y|X} \| Q_Y^* | P_X) \leq D(P_{Y|X} \| Q_Y^* | P_X^\dagger) \leq D(P_{Y|X} \| Q_Y | P_X^\dagger) \quad (138)$$

for all $P_X \in \mathcal{P}, Q_Y \in \mathcal{Q}$, where $P_X^\dagger \in \mathcal{P}^\dagger$ is a capacity-achieving input distribution, and Q_Y^* is the capacity-achieving output distribution; the minimax solution is $P_X^{(i)} = P_X^{(o)} = P_X^\dagger$; and the saddlepoint value is $D(P_{Y|X} \| Q_Y^* | P_X^\dagger) = C$. Since the higher-order terms in (137) are dominated by the first term $nD(P_{Y|X} \| P_Y^{(o)} | P_X^{(i)})$ and the second term in (137) is maximized at a dispersion-achieving P_X^* among the capacity-achieving $P_X^{(i)}, P_X^{(o)} \in \mathcal{P}^\dagger$, asymptotically, the minimax

$$\min_{P_X^{(o)} \in \mathcal{P}} \max_{P_X^{(i)} \in \mathcal{P}} \xi(P_X^{(i)}, P_X^{(o)}) \quad (139)$$

is achieved when both $P_X^{(i)}$ and $P_X^{(o)}$ are in the neighborhood of some dispersion-achieving input distribution $P_X^* \in \mathcal{P}^*$. Therefore, we fix a $P_X^* \in \mathcal{P}^*$, and consider the problem

$$\min_{P_X^{(o)}: \|P_X^{(o)} - P_X^*\| \leq \rho_n} \max_{P_X^{(i)}: \|P_X^{(i)} - P_X^*\| \leq \rho_n} \xi(P_X^{(i)}, P_X^{(o)}) \quad (140)$$

where $\rho_n \rightarrow 0$.

After taking the Taylor series expansion of $\xi(P_X^{(i)}, P_X^{(o)})$ around $(P_X^{(i)}, P_X^{(o)}) = (P_X^*, P_X^*)$, Moulin derives the asymptotic saddlepoint solution to the problem (140), which is given by [18, Lemma 14]

$$P_X^{(i)'} = P_X^* - \frac{Q^{-1}(\epsilon_n)}{2\sqrt{nV_{\epsilon_n}}} \tilde{\mathbf{v}}(P_X^*) \quad (141)$$

$$P_X^{(o)'} = P_X^* - \frac{Q^{-1}(\epsilon_n)}{2\sqrt{nV_{\epsilon_n}}} \tilde{\mathbf{v}}, \quad (142)$$

where $\mathbf{v}(P_X^*)$ and $\tilde{\mathbf{v}}$ are defined in (46)–(47), and the value of the saddlepoint is

$$\begin{aligned} \xi^*(P_X^*) &= nC - \sqrt{nV_{\epsilon_n}} Q^{-1}(\epsilon_n) \\ &+ Q^{-1}(\epsilon_n)^2 \left(\frac{\text{Sk}_u(P_X^*) \sqrt{V_{\epsilon_n}}}{6} + A_0(P_X^*) - A_1(P_X^*) \right) \\ &+ O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right) + O(1). \end{aligned} \quad (143)$$

We then turn our attention to (139). Define the set of input distributions

$$\mathcal{A} \triangleq \{P_X \in \mathcal{P}: \|P_X - P_X^*\| \leq \rho_n \text{ for some } P_X^* \in \mathcal{P}^*\} \quad (144)$$

$$\rho_n \triangleq \frac{c_0 Q^{-1}(\epsilon_n)}{\sqrt{n}}, \quad (145)$$

where $c_0 > 0$ is a constant to be determined later. We further bound (139) by setting $P_X^{(o)} = P_X^{(o)'}$ and $P_X^{(i)} = P_X^{(i)'}$ for some $P_X^* \in \mathcal{P}^*$ for the cases $P_X^{(i)} \in \mathcal{A}$ and $P_X^{(i)} \in \mathcal{A}^c$, respectively, and get

$$\begin{aligned} &\min_{P_X^{(o)} \in \mathcal{P}} \max_{P_X^{(i)} \in \mathcal{P}} \xi(P_X^{(i)}, P_X^{(o)}) \\ &\leq \max \left\{ \max_{P_X^{(i)} \in \mathcal{A}} \xi(P_X^{(i)}, P_X^{(o)'}) , \max_{P_X^{(i)} \in \mathcal{A}^c} \xi(P_X^{(i)}, P_X^*) \right\} \end{aligned} \quad (146)$$

that is, we bound the cases $P_X^{(i)} \in \mathcal{A}$ and $P_X^{(i)} \in \mathcal{A}^c$, separately.

Considering each of the dispersion-achieving input distributions $P_X^* \in \mathcal{P}^*$ and taking the Taylor series expansion of $\xi(P_X^{(i)}, P_X^{(o)'})$ around $P_X^{(i)} = P_X^{(i)'}$ give

$$\max_{P_X^{(i)} \in \mathcal{A}} \xi(P_X^{(i)}, P_X^{(o)'}) = \max_{P_X^* \in \mathcal{P}^*} \xi^*(P_X^*) + O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right). \quad (147)$$

To bound $\max_{P_X^{(i)} \in \mathcal{A}^c} \xi(P_X^{(i)}, P_X^*)$, we apply [18, Lemma 9 (iii)]⁸ and get

$$\begin{aligned} &\max_{P_X^{(i)} \in \mathcal{A}^c} \xi(P_X^{(i)}, P_X^*) \\ &\leq nC - \sqrt{nV_{\epsilon_n}} Q^{-1}(\epsilon_n) - c_1 \sqrt{n} \rho_n Q^{-1}(\epsilon_n) (1 + o(1)), \end{aligned} \quad (148)$$

where $c_1 > 0$ is a constant depending only on the channel parameters. We set the parameter c_0 so that

$$c_0 c_1 \leq \max_{P_X^* \in \mathcal{P}^*} \frac{\text{Sk}_u(P_X^*) \sqrt{V_{\epsilon_n}}}{6} + A_0(P_X^*) - A_1(P_X^*). \quad (149)$$

Combining (146)–(149), we get

$$\begin{aligned} &\min_{P_X^{(o)} \in \mathcal{P}} \max_{P_X^{(i)} \in \mathcal{P}} \xi(P_X^{(i)}, P_X^{(o)}) \leq nC - \sqrt{nV_{\epsilon_n}} Q^{-1}(\epsilon_n) \\ &+ Q^{-1}(\epsilon_n)^2 \max_{P_X^* \in \mathcal{P}^*} \left(\frac{\text{Sk}_u(P_X^*) \sqrt{V_{\epsilon_n}}}{6} + A_0(P_X^*) - A_1(P_X^*) \right) \\ &+ O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right) + O(1). \end{aligned} \quad (150)$$

We finally set the parameter δ_n in (129) so that

$$\log \delta_n = -\frac{Q^{-1}(\epsilon_n)^2}{2} - \frac{1}{2} \log n. \quad (151)$$

We expand the Taylor series of $Q^{-1}(\cdot)$ around ϵ_n using (105)–(107), and combine Lemmas 3, 4, and (150)–(151) to get (56). This completes the proof of Theorem 2.

⁸ [18] considers constant $Q^{-1}(\epsilon)$. In [18, eq. (4.7)], the third term is given as $-c_1 \sqrt{n} \rho_n$, where $Q^{-1}(\epsilon)$ is absorbed in c_1 . If we consider $Q^{-1}(\epsilon_n) \rightarrow \infty$ and carry out the same steps as [18, Lemma 9 (iii)], we see that the third term in our case becomes $-c_1 \sqrt{n} \rho_n Q^{-1}(\epsilon_n)$.

V. ASYMPTOTICS OF THE BINARY HYPOTHESIS TESTING IN THE MD REGIME

In this section, we derive the asymptotic expansion for $\beta_{1-\epsilon_n}(P^{(n)}, Q^{(n)})$ in the MD regime (6), where $P^{(n)}$ and $Q^{(n)}$ are two product distributions on a common alphabet \mathcal{X}^n . Due to [3, Th. 28], these asymptotics give a converse result for Cover-Thomas symmetric channels. In Theorem 8 in Section VI below, we prove a refined converse result that also derives the leading term of $O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right)$ in (56).

The minimum in (127) is achieved by the Neyman-Pearson Lemma (e.g., [3, Lemma 57]), i.e.,

$$P_{W|X}(0|x) = \begin{cases} 1 & \text{if } z > \gamma \\ \tau & \text{if } z = \gamma, \\ 0 & \text{if } z < \gamma \end{cases} \quad (152)$$

where $z \triangleq \log \frac{dP(x)}{dQ(x)}$ is the log-likelihood ratio, $\frac{dP(x)}{dQ(x)}$ denotes the Radon-Nikodym derivative, and τ and γ are chosen such that $\alpha = \sum_{x \in \mathcal{X}} P(x)P_{W|X}(0|x)$.

Let $P^{(n)} = \prod_{i=1}^n P_i$ and $Q^{(n)} = \prod_{i=1}^n Q_i$, where P_i and Q_i are distributions on a common alphabet \mathcal{X} . According to the meta-converse bound [3, Th. 27], the asymptotics of $\beta_\alpha(P^{(n)}, Q^{(n)})$ play a critical role in deriving a converse bound for channel coding. In [16, Lemma 14], using the Berry-Esseen Theorem, Polyanskiy *et al.* derive a third-order expansion for $\beta_\alpha(P^{(n)}, Q^{(n)})$ in the CLT regime; in [18, Th. 18], using the Edgeworth expansion and a strong large deviations theorem, Moulin proves a refinement of the asymptotics of $\beta_\alpha(P^{(n)}, Q^{(n)})$ in the CLT regime.⁹ Both of these asymptotics are used to derive tight channel coding converse bounds. Theorem 6, below, gives refined asymptotics of $\beta_\alpha(P^{(n)}, Q^{(n)})$ in the MD regime.

Theorem 6: Let P_i, Q_i be distributions on a common alphabet \mathcal{X} , and P_i be absolutely continuous with respect to Q_i for $i \in [n]$. Let $\{\epsilon_n\}_{n=1}^\infty$ be an MD sequence (6). Define $Z_i \triangleq \log \frac{dP_i(X_i)}{dQ_i(X_i)}$, where $X_i \sim P_i$ for $i \in [n]$, and

$$D_i \triangleq \mathbb{E}[Z_i] = D(P_i||Q_i) \quad (153)$$

$$V_i \triangleq \text{Var}[Z_i] = V(P_i||Q_i) \quad (154)$$

$$\mu_{k,i} \triangleq \mathbb{E}[(Z_i - D_i)^k], \quad k \geq 3 \quad (155)$$

$$\text{Sk}_i \triangleq \text{Sk}(P_i||Q_i) = \frac{\mu_{3,i}}{V_i^{3/2}} \quad (156)$$

for $i \in [n]$. Define $\bar{Z}_i \triangleq \log \frac{dP_i(\bar{Y}_i)}{dQ_i(\bar{Y}_i)}$, where $\bar{Y}_i \sim Q_i$ for $i \in [n]$, and the cumulant generating function of \bar{Z}_i

$$\kappa_i(s) \triangleq \log \mathbb{E}[\exp\{s\bar{Z}_i\}], \quad i \in [n]. \quad (157)$$

Let

$$D \triangleq \frac{1}{n} \sum_{i=1}^n D_i \quad V \triangleq \frac{1}{n} \sum_{i=1}^n V_i \quad (158)$$

$$\text{Sk} \triangleq \frac{1}{n} \sum_{i=1}^n \text{Sk}_i \quad \mu_k \triangleq \frac{1}{n} \sum_{i=1}^n \mu_{k,i}, \quad k \geq 3, \quad (159)$$

⁹There is a typo in [18, eq. (6.8)]. The sign of the third term in [18, eq. (6.8)] should be plus rather than minus.

$$\kappa(s) \triangleq \frac{1}{n} \sum_{i=1}^n \kappa_i(s). \quad (160)$$

Assume that

- (A) Z_i satisfies Cramér's condition for $i \in [n]$;
- (B) $V > 0$;
- (C) there exist positive constants β_0, β_1 , and $c > 1$ such that $\beta_0 < |\kappa(s)| < \beta_1$ for all $s \in \mathcal{D} \triangleq \{s' \in \mathbb{R}: |s'| < c\}$, and that $\kappa(s)$ is analytic in \mathcal{D} ;
- (D) if the sum $\sum_{i=1}^n \bar{Z}_i$ is non-lattice, then there exist a finite integer ℓ , a sequence $\{w_n\}_{n=1}^\infty$ satisfying $\frac{w_n}{\log n} \rightarrow \infty$, and non-overlapping index sets $\mathcal{I}_1, \mathcal{I}_2, \dots, \mathcal{I}_{w_n} \subset [n]$, each having size ℓ , such that

$$\sum_{i \in \mathcal{I}_j} \bar{Z}_i \text{ is non-lattice for } j \in [w_n]. \quad (161)$$

Then, it holds that

$$\begin{aligned} & \beta_{1-\epsilon_n}(P^{(n)}, Q^{(n)}) \\ &= \exp \left\{ - \left(nD - \sqrt{nV}Q^{-1}(\epsilon_n) + \frac{1}{2} \log n \right. \right. \\ & \quad \left. \left. + \left(\frac{\text{Sk}\sqrt{V}}{6} + \frac{1}{2} \right) Q^{-1}(\epsilon_n)^2 \right. \right. \\ & \quad \left. \left. - \frac{3(\mu_4 - 3V^2)V - 4\mu_3^2 Q^{-1}(\epsilon_n)^3}{72V^{5/2} \sqrt{n}} \right. \right. \\ & \quad \left. \left. + O\left(\frac{Q^{-1}(\epsilon_n)^4}{n} \right) + O(1) \right) \right\}. \quad (162) \end{aligned}$$

Proof: See Appendix E. ■

In Theorem 6, conditions (A) and (B) are used to apply the moderate deviations result, Lemma 1, to the sum $\sum_{i=1}^n Z_i$; conditions (C) and (D) are used to satisfy the conditions of Lemmas 4 and 5 for the random variable $\sum_{i=1}^n \bar{Z}_i$. Note that if $\sum_{i=1}^n \bar{Z}_i$ is lattice, then each of the random variables \bar{Z}_i , $i \in [n]$ is lattice. Therefore, condition (L) of Theorem 5 is satisfied for every lattice $\sum_{i=1}^n \bar{Z}_i$. In the non-lattice case, the sum $\sum_{i=1}^n \bar{Z}_i$ being non-lattice does not imply that each of \bar{Z}_i is also non-lattice. Condition (D) of Theorem 6 requires that there are $w_n \gg \log n$ non-overlapping, non-lattice partial sums of \bar{Z}_i , where each partial sum is a sum of ℓ random variables. Condition (D) is sufficient for condition (NL) of Theorem 4 to be satisfied. A condition similar to condition (D) with $\ell \leq 2$ is introduced in [18, Def. 15] for the same purpose.

VI. REFINED RESULTS FOR SYMMETRIC CHANNELS

For Cover-Thomas symmetric channels [23], it is well-known that the equiprobable distribution P_X^* on the input alphabet \mathcal{X} is the unique capacity-achieving input distribution,¹⁰ $|\mathcal{X}| = |\mathcal{Y}|$, and the capacity-achieving output distribution Q_Y^* is equiprobable on \mathcal{Y} . For Cover-Thomas symmetric channels,

- the singularity parameter $\eta(P_X^*)$ in (52) is zero, which follows by observing that for Cover-Thomas symmetric

¹⁰The uniqueness follows from the fact that the entropy of the each column of the transition matrix is equal to the entropy of the each row of the transition matrix, i.e., $H(X|Y) = H(Y|X)$.

channels, $\mathbb{E}[\iota(X; Y)|Y] = C$ almost surely and by using the law of total variation;

- the constants $A_0(P_X^*)$ and $A_1(P_X^*)$ in (49)–(50) are both equal to zero, which follows by similar steps to those in [18, Sec. III-C].

These two properties yield the skewness S in (58) for Cover-Thomas symmetric channels.

Theorem 7, below, refines the achievability result in Theorem 1 for Cover-Thomas symmetric channels.

Theorem 7: Let $P_{Y|X}$ be a Cover-Thomas symmetric channel, $V > 0$, and $\{\epsilon_n\}_{n=1}^\infty$ be an MD sequence (6). Then,

$$\begin{aligned} \zeta(n, \epsilon_n) &\geq \frac{1}{2} \log n + SQ^{-1}(\epsilon_n)^2 - \frac{3(\mu_4 - 3V^2)V - 4\mu_3^2 Q^{-1}(\epsilon_n)^3}{72V^{5/2} \sqrt{n}} \\ &\quad + O\left(\frac{Q^{-1}(\epsilon_n)^4}{n}\right) + O(1), \end{aligned} \quad (163)$$

where V and S are the dispersion and skewness under the uniform input distribution P_X^* , and $\mu_k = \mathbb{E}[(\iota(X; Y) - C)^k]$ is the k -th central moment of the information density under $X \sim P_X^*$.

Theorem 8, below, refines the converse result in Theorem 2 for Cover-Thomas symmetric channels.

Theorem 8: Under the conditions of Theorem 7,

$$\begin{aligned} \zeta(n, \epsilon_n) &\leq \frac{1}{2} \log n + SQ^{-1}(\epsilon_n)^2 - \frac{3(\mu_4 - 3V^2)V - 4\mu_3^2 Q^{-1}(\epsilon_n)^3}{72V^{5/2} \sqrt{n}} \\ &\quad + O\left(\frac{Q^{-1}(\epsilon_n)^4}{n}\right) + O(1), \end{aligned} \quad (164)$$

Proofs of Theorems 7 and 8 appear in Appendix F. Theorems 7 and 8 imply that the asymptotics in (163)–(164) are tight in the first three terms.

APPENDIX A PROOF OF LEMMA 1

Lemma 1 reduces to the Cornish-Fisher theorem when $y = O(1)$; therefore, we focus on the case $y \rightarrow \infty$ or $y \rightarrow -\infty$ with $y \in o(\sqrt{n})$. We here prove the case where $y \rightarrow \infty$. The case $y \rightarrow -\infty$ follows similarly using (65). From (66), we have

$$\begin{aligned} F_n(-x) = Q(x) \exp \left\{ -a_0 \frac{x^3}{\sqrt{n}} + a_1 \frac{x^4}{n} \right. \\ \left. - O\left(\frac{x^5}{n^{3/2}}\right) + O\left(\frac{x}{\sqrt{n}}\right) \right\}. \end{aligned} \quad (165)$$

Let $x = y + \delta$ such that $\delta/y \rightarrow 0$. As $y \rightarrow \infty$, we have the asymptotic expansion [35, eq. 26.2.12]

$$Q_Y(y) = \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{y^2}{2}\right\} \frac{1}{y} \left(1 - \frac{1}{y^2} + \frac{3}{y^4} - O\left(\frac{1}{y^6}\right)\right). \quad (166)$$

From the equation $F_n(-x) = Q(y)$, we get

$$\frac{Q_Y(y + \delta)}{Q_Y(y)}$$

$$= \exp \left\{ a_0 \frac{x^3}{\sqrt{n}} - a_1 \frac{x^4}{n} + O\left(\frac{y^5}{n^{3/2}}\right) + O\left(\frac{y}{\sqrt{n}}\right) \right\}. \quad (167)$$

Taking the logarithm of both sides of (167), we get

$$\begin{aligned} -\delta y - \frac{\delta^2}{2} - \frac{\delta}{y} + O\left(\frac{\delta^2}{y^2}\right) \\ = a_0 \frac{y^3}{\sqrt{n}} + a_0 \frac{3y^2\delta}{\sqrt{n}} + a_0 \frac{3y\delta^2}{\sqrt{n}} + a_0 \frac{\delta^3}{\sqrt{n}} - a_1 \frac{y^4}{n} \\ + O\left(\frac{y^5}{n^{3/2}}\right) + O\left(\frac{y^3\delta}{n}\right) + O\left(\frac{y}{\sqrt{n}}\right). \end{aligned} \quad (168)$$

Equating the coefficients of $\frac{y^3}{\sqrt{n}}$ and $\frac{y^4}{n}$ of both sides of (168), we get

$$b_0 = a_0 \quad (169)$$

$$b_1 = \frac{5}{2}a_0^2 + a_1, \quad (170)$$

which completes the proof.

APPENDIX B PROOF OF (116)

From (95) and (109), we get $\mathbf{a}_n \rightarrow (I(P_X), 0)$ as $n \rightarrow \infty$. To evaluate the gradient and the Hessian of $\Lambda(\mathbf{a}_n)$, we start from the equation in condition (ND)

$$\nabla \kappa(\mathbf{s}_n) = \mathbf{a}_n. \quad (171)$$

Viewing \mathbf{a}_n as a vector-valued function of \mathbf{s}_n and differentiating both sides of (171) with respect to \mathbf{s}_n , we get

$$J_{\mathbf{s}_n}(\mathbf{a}_n) = \nabla^2 \kappa(\mathbf{s}_n), \quad (172)$$

where $J_{\mathbf{s}_n}(\mathbf{a}_n) \triangleq \begin{bmatrix} \frac{\partial a_{n,1}}{\partial s_{n,1}} & \frac{\partial a_{n,1}}{\partial s_{n,2}} \\ \frac{\partial a_{n,2}}{\partial s_{n,1}} & \frac{\partial a_{n,2}}{\partial s_{n,2}} \end{bmatrix}$ is the Jacobian of \mathbf{a}_n with respect to \mathbf{s}_n .

Differentiating the equation $\Lambda(\mathbf{a}_n) = \langle \mathbf{s}_n, \nabla \kappa(\mathbf{s}_n) \rangle - \kappa(\mathbf{s}_n)$ with respect to \mathbf{s}_n , we get a 2-dimensional row vector

$$J_{\mathbf{s}_n}(\Lambda(\mathbf{a}_n)) = \mathbf{s}_n^\top \nabla^2 \kappa(\mathbf{s}_n). \quad (173)$$

Applying the function inversion theorem and using (172), we reach

$$J_{\mathbf{a}_n}(\Lambda(\mathbf{a}_n)) = J_{\mathbf{s}_n}(\Lambda(\mathbf{a}_n)) J_{\mathbf{a}_n}(\mathbf{s}_n) \quad (174)$$

$$= \mathbf{s}_n^\top \nabla^2 \kappa(\mathbf{s}_n) (\nabla^2 \kappa)^{-1}(\mathbf{s}_n) \quad (175)$$

$$= \mathbf{s}_n^\top, \quad (176)$$

equivalently

$$\nabla \Lambda(\mathbf{a}_n) = \mathbf{s}_n. \quad (177)$$

Differentiating (177) with respect to \mathbf{a}_n , we get

$$\nabla^2 \Lambda(\mathbf{a}_n) = \nabla(\nabla \Lambda(\mathbf{a}_n)) \quad (178)$$

$$= J_{\mathbf{a}_n}(\mathbf{s}_n) \quad (179)$$

$$= (\nabla^2 \kappa)^{-1}(\mathbf{s}_n). \quad (180)$$

We would like to obtain the Taylor series expansion of $\Lambda(\cdot)$ around $\mathbf{a} = (I(P_X), 0)$. By direct computation, we get

$$\Lambda(\mathbf{a}) = I(P_X) \quad (181)$$

$$\nabla \Lambda(\mathbf{a}) = (1, 1) \quad (182)$$

$$\nabla \kappa((1, 1)) = \mathbf{a}, \quad (183)$$

giving $\mathbf{s}_n \rightarrow \mathbf{s} \triangleq (1, 1)$, which verifies condition (ND). Define

$$\mathbf{T} \triangleq (T_1, T_2) \quad (184)$$

$$T_1 \triangleq \log \frac{P_{Y|X}(Y|X)}{P_Y(Y)} \quad (185)$$

$$T_2 \triangleq \log \frac{P_{Y|X}(Y|\bar{X})}{P_{Y|X}(Y|X)}, \quad (186)$$

where $P_{X, \bar{X}, Y}(x, \bar{x}, y) = P_X(x)P_X(\bar{x})P_{Y|X}(y|x)$. We have

$$\nabla^2 \kappa(\mathbf{s}) = \text{Cov}(\tilde{\mathbf{T}})^{-1}, \quad (187)$$

where $\tilde{\mathbf{T}}$ is distributed according to the tilted distribution

$$P_{\tilde{\mathbf{T}}} = \exp\{\langle \mathbf{s}, \mathbf{T} \rangle\} P_{\mathbf{T}} = \frac{P_{Y|X}(Y|\bar{X})}{P_Y(Y)} P_{\mathbf{T}}, \quad (188)$$

and $P_{\mathbf{T}}$ denotes the distribution of \mathbf{T} . We compute the inverse of the covariance matrix of $\tilde{\mathbf{T}}$ as

$$\text{Cov}(\tilde{\mathbf{T}})^{-1} = \begin{bmatrix} \frac{2}{1+\eta(P_X)} & \frac{1}{1+\eta(P_X)} \\ \frac{1}{1+\eta(P_X)} & \frac{1}{1-\eta(P_X)^2} \end{bmatrix} \frac{1}{V_u(P_X)}. \quad (189)$$

From (181), (182), and (189), we get

$$\begin{aligned} \Lambda(\mathbf{a}_n) &= I(P_X) + (a_{n,1} - I(P_X)) \\ &\quad + \frac{1}{2}(a_{n,1} - I(P_X))^2 \text{Cov}(\tilde{\mathbf{T}})_{1,1}^{-1} + O(|a_{n,1} - I(P_X)|^3) \\ &= a_{n,1} + \frac{1}{n} \frac{Q^{-1}(\epsilon_n)^2}{1 + \eta(P_X)} + O\left(\frac{Q^{-1}(\epsilon_n)^3}{n^{3/2}}\right) + O\left(\frac{1}{n}\right). \end{aligned} \quad (190) \quad (191)$$

APPENDIX C PROOF OF (124)

We solve the convex optimization problem in (123) by writing the Lagrangian

$$L(\mathbf{g}, \lambda) = \mathbf{g}^\top \mathbf{h} - \frac{1}{2} \mathbf{g}^\top \mathbf{J} \mathbf{g} - \lambda \mathbf{g}^\top \mathbf{1}. \quad (192)$$

The Karush-Kuhn-Tucker condition $\nabla L(\mathbf{g}, \lambda) = 0$ gives

$$\mathbf{J} \mathbf{g} = \mathbf{h} - \lambda \mathbf{1} \quad (193)$$

$$\mathbf{g}^\top \mathbf{1} = 0, \quad (194)$$

where \mathbf{J} is given in (41). The equation (193) has a solution since both \mathbf{h} and $\mathbf{1}$ are in the row space of \mathbf{J} , which is equal to the column space since \mathbf{J} is symmetric. Solving the system of equations in (193) and (194), we get the dual variable

$$\lambda^* = \frac{\mathbf{1}^\top \mathbf{J} \mathbf{h}}{\mathbf{1}^\top \mathbf{J} \mathbf{1}}. \quad (195)$$

Plugging (195) in (194), we get

$$\mathbf{g}^* = \tilde{\mathbf{J}} \mathbf{h} \quad (196)$$

$$= -\frac{Q^{-1}(\epsilon_n)}{2\sqrt{n}V_{\epsilon_n}} \tilde{\mathbf{J}} \mathbf{v}(P_X^*), \quad (197)$$

where $\tilde{\mathbf{J}}$ and \mathbf{v} are given in (45) and (46). An equivalent characterization of (197) in terms of the eigenvalue decomposition of \mathbf{J} is given in [18, Lemma 1 (v)]. The value of the supremum in (123) is $\frac{1}{2} \mathbf{g}^{*\top} \mathbf{J} \mathbf{g}^* = A_0(P_X^*) Q^{-1}(\epsilon_n)^2$, where $A_0(\cdot)$ is given in (49).

APPENDIX D PROOF OF LEMMA 4

We compute the first 3 central moments of the random variable $\sum_{i=1}^n \log \frac{P_{Y|X}(Y_i|x_i)}{Q_Y(Y_i)}$, where $\mathbf{Y} \sim P_{\mathbf{Y}|\mathbf{X}=\mathbf{x}}$, which is the sum of n independent, but not necessarily identical random variables. We have

$$\begin{aligned} &\frac{1}{n} \mathbb{E} \left[\sum_{i=1}^n \log \frac{P_{Y|X}(Y_i|x_i)}{Q_Y(Y_i)} \right] \\ &= \sum_{y \in \mathcal{Y}} \sum_{\tilde{x} \in \mathcal{X}} \hat{P}_{\mathbf{x}}(\tilde{x}) P_{Y|X}(y|\tilde{x}) \log \frac{P_{Y|X}(y|\tilde{x})}{Q_Y(y)} \end{aligned} \quad (198)$$

$$= D_{\mathbf{x}}. \quad (199)$$

Similarly, it follows that

$$\frac{1}{n} \text{Var} \left[\sum_{i=1}^n \log \frac{P_{Y|X}(Y_i|x_i)}{Q_Y(Y_i)} \right] = V_{\mathbf{x}} \quad (200)$$

$$\mathbb{E} \left[\left(\frac{1}{n} \sum_{i=1}^n \log \frac{P_{Y|X}(Y_i|x_i)}{Q_Y(Y_i)} - D_{\mathbf{x}} \right)^3 \right] = T_{\mathbf{x}}. \quad (201)$$

Note that Cramér's condition in Theorem 3 is satisfied since $\log \frac{P_{Y|X}(Y_i|x_i)}{Q_Y(Y_i)}$ is a discrete random variable for all $i \in [n]$.

Applying Lemma 1 by setting X_i to $\log \frac{P_{Y|X}(Y_i|x_i)}{Q_Y(Y_i)}$ gives (133).

APPENDIX E PROOF OF THEOREM 6

Assume that $\sum_{i=1}^n Z_i$ is lattice with a span $h > 0$. Let $\underline{\gamma}$ and $\bar{\gamma}$ satisfy

$$\mathbb{P} \left[\sum_{i=1}^n Z_i \geq \underline{\gamma} \right] = 1 - \underline{\epsilon}_n \geq 1 - \epsilon_n \quad (202)$$

$$\mathbb{P} \left[\sum_{i=1}^n Z_i \geq \bar{\gamma} \right] = 1 - \bar{\epsilon}_n \leq 1 - \epsilon_n, \quad (203)$$

where $\underline{\gamma}$ and $\bar{\gamma}$ are in the range of $\sum_{i=1}^n Z_i$, $\bar{\gamma} - \underline{\gamma} = h$, and $\underline{\epsilon}_n \leq \epsilon_n \leq \bar{\epsilon}_n$. Let $\lambda \in [0, 1]$ satisfy

$$\mathbb{P} \left[\sum_{i=1}^n Z_i \geq \underline{\gamma} \right] \lambda + \mathbb{P} \left[\sum_{i=1}^n Z_i \geq \bar{\gamma} \right] (1 - \lambda) = 1 - \epsilon_n. \quad (204)$$

By the Neyman-Pearson Lemma (see [3, eq. (101)]),

$$\begin{aligned} &\beta_{1-\epsilon_n}(P^{(n)}, Q^{(n)}) \\ &= \mathbb{P} \left[\sum_{i=1}^n \bar{Z}_i \geq \underline{\gamma} \right] \lambda + \mathbb{P} \left[\sum_{i=1}^n \bar{Z}_i \geq \bar{\gamma} \right] (1 - \lambda). \end{aligned} \quad (205)$$

Define the asymptotic expansion

$$\begin{aligned} \chi(\epsilon) &\triangleq D - \sqrt{\frac{V}{n}} Q^{-1}(\epsilon) + \frac{\text{Sk} \sqrt{V}}{6n} Q^{-1}(\epsilon)^2 \\ &\quad - \frac{3(\mu_4 - 3V^2)V - 4\mu_3^2}{72V^{5/2}} \frac{Q^{-1}(\epsilon)^3}{n^{3/2}} \\ &\quad + O\left(\frac{Q^{-1}(\epsilon)^4}{n^2}\right) + O\left(\frac{1}{n}\right). \end{aligned} \quad (206)$$

By conditions (A) and (B) of Theorem 6, the conditions of Theorem 3 are satisfied for the sum $\sum_{i=1}^n Z_i$. We apply Lemma 1 to (202)–(203), and get the asymptotic expansions

$$\underline{\gamma} = n\chi(\underline{\epsilon}_n) \quad (207)$$

$$\bar{\gamma} = n\chi(\bar{\epsilon}_n). \quad (208)$$

From the Taylor series expansion of $\chi(\cdot)$ around ϵ_n , (207)–(208), and $\bar{\gamma} - \underline{\gamma} = O(1)$, it holds that

$$\underline{\gamma} = n\chi(\epsilon_n) + O(1) \quad (209)$$

$$\bar{\gamma} = n\chi(\epsilon_n) + O(1). \quad (210)$$

The arguments above hold in the non-lattice case with $\underline{\gamma} = \bar{\gamma}$.

Next, we evaluate the probability $\mathbb{P}[\sum_{i=1}^n \bar{Z}_i \geq \underline{\gamma}]$ in (205) separately in the lattice and non-lattice cases.

1) *Lattice case*: We will apply Theorem 5 to evaluate the probability of interest. By [18, Appendix D],

$$\kappa(1) = 0 \quad (211)$$

$$\kappa'(1) = D \quad (212)$$

$$\kappa''(1) = V \quad (213)$$

$$\kappa'''(1) = \mu_3. \quad (214)$$

From (209), we have $\frac{1}{n}\underline{\gamma} = D + o(1)$. Therefore, by (212), condition (ND) of Theorem 4 is satisfied with $s = 1 + o(1)$. Condition (S) of Theorem 4 is satisfied by condition (C) of Theorem 6. Therefore, it only remains to verify condition (L) of Theorem 5 in the one-dimensional case. Since $\sum_{i=1}^n \bar{Z}_i$ is lattice with span h , each of \bar{Z}_i is also lattice with a span multiple of h . By [32, p. 1687], we have

$$\sup_{\delta < |t| \leq \frac{\pi}{h}} \left| \frac{\phi_i(s+it)}{\phi_i(s)} \right| \leq c_1 < 1, \quad i \in [n] \quad (215)$$

for every $0 < \delta \leq \frac{\pi}{h}$, where $\phi_i(\cdot)$ is the MGF of \bar{Z}_i . Since $\bar{Z}_1, \dots, \bar{Z}_n$ are i.i.d., the MGF $\phi(\cdot)$ of $\sum_{i=1}^n \bar{Z}_i$ satisfies

$$\sup_{\delta < |t| \leq \frac{\pi}{h}} \left| \frac{\phi(s+it)}{\phi(s)} \right| = \sup_{\delta < |t| \leq \frac{\pi}{h}} \left| \prod_{i=1}^n \frac{\phi_i(s+it)}{\phi_i(s)} \right| \quad (216)$$

$$\leq c_1^n = o(n^{1/2}). \quad (217)$$

Therefore, condition (L) of Theorem 5 is satisfied. Applying Theorem 5 to $\mathbb{P}[\sum_{i=1}^n \bar{Z}_i \geq \underline{\gamma}]$, we have

$$\mathbb{P}\left[\sum_{i=1}^n \bar{Z}_i \geq \underline{\gamma}\right] = \exp\left\{-n\Lambda(a_n) - \frac{1}{2}\log n + O(1)\right\}, \quad (218)$$

where

$$\Lambda(a_n) = \sup_{t \in \mathbb{R}} \{ta_n - \kappa(t)\} \quad (219)$$

$$a_n = \chi(\epsilon_n) + O\left(\frac{1}{n}\right). \quad (220)$$

We expand the Taylor series of $\Lambda(\cdot)$ around D as

$$\begin{aligned} \Lambda(a_n) &= \Lambda(D) + (a_n - D)\Lambda'_n(D) + \frac{(a_n - D)^2}{2}\Lambda''_n(D) \\ &\quad + \frac{(a_n - D)^3}{6}\Lambda'''_n(D) + O(|a_n - D|^4). \end{aligned} \quad (221)$$

By [18, Appendix D],

$$\Lambda(D) = D \quad (222)$$

$$\Lambda'_n(D) = 1 \quad (223)$$

$$\Lambda''_n(D) = \frac{1}{V} \quad (224)$$

$$\Lambda'''_n(D) = -\frac{\mu_3}{V^3}. \quad (225)$$

Combining (218) and (222)–(225), we get

$$\Lambda(a_n) = a_n + \frac{Q^{-1}(\epsilon_n)^2}{2n} + O\left(\frac{Q^{-1}(\epsilon_n)^4}{n^2}\right) + O\left(\frac{1}{n}\right). \quad (226)$$

By (209)–(210), the asymptotic expansion on the right-hand side of (218) holds for the probability $\mathbb{P}[\sum_{i=1}^n \bar{Z}_i \geq \bar{\gamma}]$. Combining (205), (218), and (226) completes the proof for the lattice case.

2) *Non-lattice case*: The proof for the non-lattice is identical to the proof for the lattice case except the verification of condition (NL) in Theorem 4. Denote

$$\tilde{S}_j \triangleq \sum_{i \in \mathcal{I}_j} Z_i, \quad j \in [w_n], \quad (227)$$

which are non-lattice by condition (D) of Theorem 6. By [32, p. 1687],

$$\sup_{j \in [w_n]} \sup_{\delta < |t| \leq \lambda} \left| \frac{\tilde{\phi}_j(s+it)}{\tilde{\phi}_j(s)} \right| \leq c_2 < 1 \quad (228)$$

for every $0 < \delta < \lambda$, where $\tilde{\phi}_j$ denotes the MGF of \tilde{S}_j . Since $\bar{Z}_1, \dots, \bar{Z}_n$ are i.i.d., we have

$$\sup_{\delta < |t| \leq \lambda} \left| \frac{\phi(s+it)}{\phi(s)} \right| = \sup_{\delta < |t| \leq \lambda} \left| \prod_{j=1}^{w_n} \frac{\tilde{\phi}_j(s+it)}{\tilde{\phi}_j(s)} \right| \cdot 1 \quad (229)$$

$$\leq c_2^{w_n} \quad (230)$$

$$= o(n^{1/2}), \quad (231)$$

where (229) follows since $\frac{\tilde{\phi}_j(s+it)}{\tilde{\phi}_j(s)}$ is a characteristic function of a non-lattice random variable [32], (230) follows from (228), and (231) follows from condition (D) and $c_2 < 1$. This verifies condition (NL) of Theorem 4. Applying Theorem 4 similarly to (218) completes the proof.

APPENDIX F PROOFS OF THEOREMS 7 AND 8

Proof of Theorem 7: To prove Theorem 7, we derive the coefficient of $O\left(\frac{Q^{-1}(\epsilon_n)^3}{\sqrt{n}}\right)$ in Lemma 2, and invoke the refined Lemma 2 with $P_X = P_X^*$. For this purpose, we need to modify the proof of Lemma 2 at two steps. First, using Lemma 1, the expansion for t_n in (108) is refined as

$$\begin{aligned} t_n &= Q^{-1}(\epsilon_n) - \frac{\text{Sk}_u Q^{-1}(\epsilon_n)^2}{6\sqrt{n}} \\ &\quad - \frac{3(\mu_4 - 3V^2)V - 4\mu_3^2}{72V^3} \frac{Q^{-1}(\epsilon_n)^3}{n} \\ &\quad + O\left(\frac{Q^{-1}(\epsilon_n)^4}{n^{3/2}}\right) + O\left(\frac{1}{\sqrt{n}}\right). \end{aligned} \quad (232)$$

Second, we refine the expansion in (116) by computing the third-order gradient $\nabla^3 \Lambda(\mathbf{a}_n)$. Taking the gradient of (180), we get

$$\begin{aligned} & \nabla^3 \Lambda(\mathbf{a}_n)_{i,j,k} \\ &= - \sum_{(a,b,c) \in [2]^3} \nabla^3 \kappa_{a,b,c}(\mathbf{s}_n) (\nabla^2 \kappa)_{a,i}^{-1}(\mathbf{s}_n) (\nabla^2 \kappa)_{b,j}^{-1}(\mathbf{s}_n) \\ & \quad \cdot (\nabla^2 \kappa)_{c,k}^{-1}(\mathbf{s}_n), \quad (i,j,k) \in [2]^3. \end{aligned} \quad (233)$$

In the case that $\eta(P_X^*) = 0$, $(\nabla^2 \kappa)^{-1}(\mathbf{s})$ in (187) becomes

$$(\nabla^2 \kappa)^{-1}(\mathbf{s}) = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix} \frac{1}{V}, \quad (234)$$

and we compute

$$\nabla^3 \kappa(\mathbf{s})_{1,1,1} = \mu_3 \quad (235)$$

$$\nabla^3 \kappa(\mathbf{s})_{1,1,2} = -\mu_3 \quad (236)$$

$$\nabla^3 \kappa(\mathbf{s})_{1,2,2} = \mu_3 \quad (237)$$

$$\nabla^3 \kappa(\mathbf{s})_{2,2,2} = 0. \quad (238)$$

Note that (235)–(238) is sufficient to determine $\nabla^3 \kappa(\mathbf{s})$ since it is a symmetric order-3 tensor. From (233)–(238), we compute

$$\nabla^3 \Lambda(\mathbf{a})_{1,1,1} = -\frac{2\mu_3}{V^3}. \quad (239)$$

Using (234) and (239), we refine (116) as

$$\begin{aligned} \Lambda(\mathbf{a}_n) &= a_{n,1} + \frac{(a_{n,1} - I(P_X^*))^2}{V} - \frac{1}{6}(a_{n,1} - I(P_X^*))^3 \frac{2\mu_3}{V^3} \\ & \quad + O(|a_{n,1} - I(P_X^*)|^4) \quad (240) \\ &= a_n + \frac{Q^{-1}(\epsilon_n)^2}{n} + O\left(\frac{Q^{-1}(\epsilon_n)^4}{n^2}\right) + O\left(\frac{1}{n}\right). \end{aligned} \quad (241)$$

Following the steps in the proof Lemma 2 and using (232) and (241) completes the proof. ■

Proof of Theorem 8: Set $Q_Y^{(n)} = (Q_Y^*)^n$, where Q_Y^* is the equiprobable capacity-achieving output distribution. Since Cover-Thomas symmetric channels have rows that are permutation of each other, we have that $\beta_{1-\epsilon_n}(P_{Y|X=\mathbf{x}}, Q_Y^{(n)})$ is independent of $\mathbf{x} \in \mathcal{X}^n$. By [3, Th. 28], we have

$$\log M^*(n, \epsilon_n) \leq -\log \beta_{1-\epsilon_n}(P_{Y|X=\mathbf{x}}, Q_Y^{(n)}), \quad (242)$$

where $\mathbf{x} = (x_0, \dots, x_0)$ for some $x_0 \in \mathcal{X}$. Applying Theorem 6 to the right-hand side of (242) completes the proof. ■

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