Matrix Poincaré, Φ -Sobolev Inequalities, and Quantum Ensembles

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ABSTRACT. Sobolev-type inequalities have been extensively studied in the frameworks of real-valued functions and non-commutative \mathbb{L}_p spaces, and have proven useful in bounding the time evolution of classical/quantum Markov processes, among many other applications. In this paper, we consider yet another fundamental setting — matrix-valued functions — and prove new Sobolev-type inequalities for them. Our technical contributions are two-fold: (i) we establish a series of matrix Poincaré inequalities for separably convex functions and general functions with Gaussian unitary ensembles inputs; and (ii) we derive Φ -Sobolev inequalities for matrix-valued functions defined on Boolean hypercubes and for those with Gaussian distributions. Our results recover the corresponding classical inequalities (i.e. real-valued functions) when the matrix has one dimension. Finally, as an application of our technical outcomes, we derive the upper bounds for a fundamental entropic quantity — the Holevo quantity — in quantum information science since classical-quantum channels are a special instance of matrix-valued functions. This is obtained through the equivalence between the constants in the strong data processing inequality and the Φ -Sobolev inequality.

1. INTRODUCTION

Sobolev-type inequalities generally refer to upper bounding the uncertainty of real-valued functions $f : \mathcal{X} \to \mathbb{R}$ by its Dirichlet energy, while the hypercontractive inequality indicates upper bounding the lower moment of f by its higher moment. These functional inequalities were originally motivated by the study of the semiboundedness of certain quantum field Hamiltonians [1]. Substantial progress was independently made by several authors in the 1970's [2, 3, 4, 5] (see also the review literature [6, 7, 8, 9, 10, 11, 12]). In particular, Federbush proved that the logarithmic Sobolev (log-Sobolev) inequality implies the hypercontractivity [13]. Later, Gross' groundbreaking work [14] showed the equivalence between the log-Sobolev inequality and the hypercontractive inequality.

Since then, log-Sobolev inequalities have become a rich topic that has influenced numerous areas of research [15, 16, 17, 11]. For example, hypercontractivity was applied to bounding the local influence of Boolean functions through a global variation in theoretical computer science [18, 19, 20]. In physics, the Poincaré and log-Sobolev inequalities provide useful tools for characterising the time evolution of dynamical systems. The convergence rate of a Markov process to its equilibrium can thus be determined by the constants of the Sobolev inequalities [21, 22, 10, 12].

Motivated by the studies of quantum fermion fields [3, 23, 24], recent research interest has switched to these functional inequalities in the non-commutative setting. In the late 20th century, Olkiewicz and Zegarlinski completed a crucial step by generalising Gross' log-Sobolev inequalities [14] in non-commutative L_p space, and proved their equivalence with hypercontractivity under some regular conditions [25]. New results and progress has thus emerged in this line of research [26, 27, 28, 29, 30] (see also [31] and the references therein). Specifically, noncommutative log-Sobolev inequalities enable the analysis of the dynamics of von Neumann algebras, including their most interesting case — the time evolution of a single quantum state through a Markov process [32]. Kastoryano and Temme derived mixing time bounds in some quantum channel semigroups [33]. The exponential decay phenomena of various entropic quantities were later discovered [34, 35, 33, 36, 37, 38, 39]. Moreover, the equivalence of log-Sobolev inequalities and hypercontractivity for completely bounded norms of quantum channel semigroups was proven under certain assumptions [40, 41].

Although commutative and noncommutative Sobolev-type inequalities have succeeded in characterising the dynamics of classical and quantum Markov systems, these functional inequalities cannot be applied to another fundamental scenario — the time evolution of an ensemble of matrices. This scenario includes classical-quantum channels as a special case; hence, it plays a substantial role in quantum information processing and communication tasks since investigating the dynamics of a quantum ensemble would enable us to capture the information capability of a communication or computation process [42]. In this paper, we pioneer the study of Sobolev-type inequalities in the framework of ensemble matrices, and establish the corresponding matrix Poincaré, Φ -Sobolev, and log-Sobolev inequalities. Our result can be viewed as a direct generalisation of real-valued functions f in classical inequalities with matrix-valued functions $f: \mathcal{X} \to \mathbb{C}^{d \times d}$. Consequently, we can recover the classical case when d = 1. Furthermore, we give a partial answer to the equivalence between hypercontractivity and the log-Sobolev inequality; we show that the matrix Bonami-Gross-Beckner inequality by Ben-Aroya et al. [19] implies the proposed matrix Φ -Sobolev inequality. As an application, we show how the Holevo quantity of a quantum ensemble changes as it evolves according to a classical Markov kernel on its classical labels and a post-selection rule.

The proposed generalisations could have potential impacts in other research areas as well. For example, in many branches of science and engineering, observed data are more efficiently represented as matrices, such as Dyson's model of matrix-valued Brownian motion [43], collaborative filtering [44], group Lasso [45], and multi-class learning [46]. Thus, system performance can be determined through analysis if a random assumption is placed on the matrices [47]. A recent review of modern random matrix concentration theory surveyed the most successful methods from these topics and provided interesting examples that these techniques can illuminate [48, 49, 50].

1.1. Our Results. The contributions of this paper are two-fold.

- (1) We derive various functional inequalities, including matrix Poincaré inequalities, matrix Sobolev inequalities, and matrix log-Sobolev inequalities.
 - We prove a Poincaré inequality for matrix-valued functions in Theorem 2 (see also Corollary 3), which generalises the classical Poincaré inequality [51, 52]:

$$\operatorname{Var}(f(X)) \le \mathbb{E}\left[\|\nabla f(X)\|^2 \right],\tag{1}$$

where $X \triangleq (X_1, \ldots, X_n)$ denotes an independent random vector with each X_i taking values in the interval [0, 1]. Our proof, paralleling its classical counterpart, relies on the matrixvalued Efron-Stein inequality (Theorem 1). Both Theorem 2 and Corollary 3 recover the classical Poincaré inequality (1) when the matrix dimension d = 1. We also derive Poincaré inequalities for matrix-valued functions with additional assumptions of pairwise commutation (Corollary 3). Finally, we derive a matrix Gaussian Poincaré inequality for Gaussian unitary ensembles (Theorem 4).

- We prove a Φ -Sobolev inequality for matrix-valued functions defined on the Boolean hypercube in Theorem 6, from which we can extend to a Φ -Sobolev inequality for Gaussian distributions (Theorem 7). Our Φ -Sobolev inequality is defective (see Remark 3.2 for a discussion on *tight* and *defective* Φ -Sobolev inequalities), but again it recovers the classical Φ -Sobolev inequality when d = 1. Our proof builds upon a powerful matrix Bonami-Gross-Beckner inequality [19], from which the hypercontractivity inequality for matrix-valued functions on Boolean hypercubes can be obtained. The matrix log-Sobolev inequalities in Corollaries 8 and 9 follow immediately from Theorems 6 and 7.
- (2) Finally, we connect matrix Φ -entropies to quantum information theory. When $\Phi(x) = x \log x$ and the random matrix $\rho_X \equiv \{p(x), \rho_x\}_{x \in \mathcal{X}}$, where each $\rho_x \succeq 0$ and $\operatorname{Tr} \rho_x = 1$ is a quantum ensemble, $H_{\Phi}(\rho_X)$ is equal to the Holevo quantity $\chi(\{p, \rho\})$ (up to a constant dimensional factor for purely technical purposes). If the ensemble $\rho_Y \equiv \{q(y), \sigma_y\}_{y \in \mathcal{Y}}$ is obtained by evolving ρ_X with a Markov kernel K(y|x):

$$q(y) = \sum_{x} p(x)K(y|x), \text{ and } \sigma_y = \sum_{x} \rho_x K^*(x|y)$$

where $K^*(x|y)$ is the backward channel of K, then the Holevo quantity of $\chi(\{p, \rho\})$ is bounded from above by a constant c times the average Holevo quantity of the ensembles that come from post-selecting the original $\{p, \rho\}$ by the postselection rule K^* . Moreover, the constant c is related to the ratio of the Holevo quantities $\chi(\{p, \rho\})$ and $\chi(\{q, \sigma\})$ (see Proposition 10). This bears a stronger form of the classical strong data processing inequality [53, 17].

1.2. Prior work.

- (1) Very few matrix concentration results have been established for general matrix-valued functions. To the best of our knowledge, the only gem in this area is a family of polynomial Efron-Stein inequalities for random matrices [54], where the theory of exchangeable pairs is used in the proof. In a previous work, we proved the subadditivity property of operator-valued Φ -entropies, and derived an operator Efron-Stein inequality (see also Theorem 1).
- (2) We would also like to point out that the matrix Φ -entropies defined in the paper are different from the entropy functions in the non-commutative \mathbb{L}_p spaces discussed in [23, 24, 19, 20, 35, 33, 40, 36]. Hence, our functional inequalities in Section 3 are incomparable with those in the non-commutative \mathbb{L}_p spaces.

This paper is organised as follows: Section 2 reviews the matrix algebra necessary for the remaining paper. We derive Sobolev-type inequalities for matrix-valued functions in Section 3. We connect matrix Φ -entropies to quantum information theory and derive an upper bound for the Holevo quantity in Section 4. Conclusions are given in Section 5. Appendix A collects useful lemmas.

2. Preliminaries

In this section we present the background information necessary for this paper. Basic notations are introduced in Section 2.1. We then review operator algebra with a focus on *Fréchet derivatives* and the convexity properties of matrix-valued functions in Section 2.2 and 2.3, respectively.

2.1. Notation. Given a separable Hilbert space \mathcal{H} , denote by \mathbb{M} the Banach space of all linear operators on \mathcal{H} . The set \mathbb{M}^{sa} refers to the subspace of the self-adjoint operators in \mathbb{M} . We denote by \mathbb{M}^+ (resp. \mathbb{M}^{++}) the set of positive semi-definite (resp. positive-definite) operators in \mathbb{M}^{sa} . If the dimension d of a Hilbert space \mathcal{H} needs special attention, it is highlighted in subscripts, e.g., \mathbb{M}_d denotes the Banach space of $d \times d$ complex matrices. The trace function $\operatorname{Tr} : \mathbb{M} \to \mathbb{C}$ is defined as $\operatorname{Tr}[M] \triangleq \sum_k e_k^* M e_k$ for $M \in \mathbb{M}$, where $(e_k)_k$ is any orthonormal basis of \mathcal{H} . If we focus on finite dimensional Hilbert spaces, then the trace function acting on M is equal to the sum of its eigenvalues. In this paper, we introduce a normalised trace function $\overline{\operatorname{tr}}$ for every matrix $M \in \mathbb{M}_d$ as $\overline{\operatorname{tr}}[M] \triangleq \frac{1}{d} \operatorname{Tr}[M]$. For $p \in [1, \infty)$, the Schatten p-norm of an operator $M \in \mathbb{M}^{sa}$ is denoted as $\|M\|_p \triangleq (\operatorname{Tr}|M|^p)^{1/p}$, where $|M| \triangleq \sqrt{M^2}$.

We define \mathbb{S}^n as the set of all mutually commuting *n*-tuple self-adjoint operators; namely, if $\vec{X} = (X_1, \ldots, X_n) \in \mathbb{S}^n$, then $[X_i, X_j] = 0$ for $i \neq j \in \{1, \ldots, n\}$. We denote by \mathbb{S}^n_d the set of mutually commuting *n*-tuple $d \times d$ Hermitian matrices. For $A, B \in \mathbb{M}^{sa}$, $A \succeq B$ means that A - B is positive semi-definite. Similarly, $A \succ B$ means A - B is positive-definite. We denote by $A \preceq_U B, A, B \in \mathbb{M}_d^{sa}$ when $\sigma_i(A) \leq \sigma_i(B), i = 1, \ldots, d$, where $\sigma(A) \triangleq (\sigma_1(A), \ldots, \sigma_d(A))$ are the eigenvalues of A arranged in decreasing order.

Throughout this paper, italic capital letters (e.g. \mathbf{X}) are used to denote operators and the underlined italic capital letters (e.g., \mathbf{X}) are used to denote a vector of, say n, operators.

2.2. Matrix Calculus. In this section, we only provide information relating to the matrix calculus. For a general treatment of this topic, please refer to [55, Section 2.1], [56, Chapter 17], [57, Section X.4], [58, Section 5.3], and [59, Chapter 3].

Let \mathcal{U}, \mathcal{W} be real Banach spaces. The Fréchet derivative of a function $f : \mathcal{U} \to \mathcal{W}$ at a point $X \in \mathcal{U}$, if it exists¹, is a unique linear mapping $\mathsf{D}f[X] : \mathcal{U} \to \mathcal{W}$ such that

$$\frac{\|\boldsymbol{f}(\boldsymbol{X}+\boldsymbol{E})-\boldsymbol{f}(\boldsymbol{X})-\mathsf{D}\boldsymbol{f}[\boldsymbol{X}](\boldsymbol{E})\|_{\mathcal{W}}}{\|\boldsymbol{E}\|_{\mathcal{U}}}\to 0 \quad \text{as } \boldsymbol{E}\in\mathcal{U} \ \text{and} \ \|\boldsymbol{E}\|_{\mathcal{U}}\to\boldsymbol{0}.$$

The Fréchet derivative also satisfies the sum rule, the product rule, and the chain rule as in the conventional derivatives of real-valued functions (see e.g. [59, Theorem 3.4]).

 $^{^{1}}$ We assume the functions considered in the paper are Fréchet differentiable. We refer readers to works, such as [60, 61] for the conditions under which a function is Fréchet differentiable.

The partial Fréchet derivative of multivariate functions can be defined as follows [58, Section 5.3]. Let \mathcal{U}, \mathcal{V} and \mathcal{W} be real Banach spaces, $f: \mathcal{U} \times \mathcal{V} \to \mathcal{W}$. For a fixed $v_0 \in \mathcal{V}$, $f(u, v_0)$ is a function of u whose derivative at u_0 , if it exists, is called the partial Fréchet derivative of f with respect to u, and is denoted by $D_u f[u_0, v_0]$. The partial Fréchet derivative $D_v f[u_0, v_0]$ is defined similarly.

For any map $f : \mathcal{U} \to \mathcal{W}$ and an operator $X \in \mathcal{U}$, we define the induced norm of the Fréchet derivative $\mathsf{D}f[X]$ as

$$\|\mathsf{D}\boldsymbol{f}[\boldsymbol{X}]\| \triangleq \sup_{\boldsymbol{E}\neq\boldsymbol{0}} \frac{\|\mathsf{D}\boldsymbol{f}[\boldsymbol{X}](\boldsymbol{E})\|}{\|\boldsymbol{E}\|},\tag{2}$$

where the norm can be any consistent norm (e.g. $\|\mathsf{D}f[X]\|_2 = \sup_{E\neq 0} \|\mathsf{D}f[X](E)\|_2 / \|E\|_2$).

2.3. Standard Matrix Functions. For each self-adjoint and bounded operator $\mathbf{A} \in \mathbb{M}^{sa}$ with the spectral decomposition $\mathbf{A} = \int_{\lambda \in \sigma(\mathbf{A})} \lambda \, \mathrm{d}\mathbf{E}(\lambda)$, we define the *standard matrix function* of each scalar function by $f(\mathbf{A}) \triangleq \int_{\lambda \in \sigma(\mathbf{X})} f(\lambda) \, \mathrm{d}\mathbf{E}(\lambda)$. Note that we use lowercase Roman and Greek letters to denote standard matrix functions, while the calligraphic capital letter \mathbf{f} refers to general operator-valued functions that are not necessarily standard.

A function $f : \mathbb{R} \to \mathbb{R}$ is called *operator convex* if for each $A, B \in \mathbb{M}^{sa}$ and $0 \le t \le 1$, $f(tA + (1 - t)B) \le tf(A) + (1 - t)f(B)$. Similarly, a function f is called *operator monotone* if, for each $A, B \in \mathbb{M}^{sa}$, $A \le B \Rightarrow f(A) \le f(B)$.

The standard matrix function can be extended into the multivariate case by considering n-tuples commuting self-adjoint operators, i.e.

$$f(\vec{\boldsymbol{X}}) \triangleq \int_{(\lambda_1,\dots,\lambda_n)} f(\lambda_1,\dots,\lambda_n) \,\mathrm{d}\boldsymbol{E}(\lambda_1,\dots,\lambda_n).$$
(3)

for $\vec{X} = (X_1, \ldots, X_n) \in \mathbb{S}^n$ with $X_i = \int_{\lambda} \lambda dE_i(\lambda)$ and $E(\lambda_1, \ldots, \lambda_n) \triangleq E(\lambda_1) \cdots E(\lambda_n)$. Define the (first-order) divided difference of the multivariate matrix function $f : \mathbb{R}^n \to \mathbb{R}$, for each $i = 1, \ldots, n$, by using the rule:

$$\varphi_i(\bar{x},\bar{y}) = \frac{(f(\bar{x}-\bar{y}))(x_i-y_i)}{\|\bar{x}-\bar{y}\|_2^2} \text{ for } \bar{x} \neq \bar{y} \text{ and } \varphi_k(\bar{x},\bar{x}) = \frac{\partial f}{\partial x_i}(\bar{x}), \tag{4}$$

where $\bar{x} \triangleq (x_1, \ldots, x_n) \in \mathbb{R}^n$. A multivariate extension of the Daleckiĭ and Kreĭn formula [59, Theorem 3.11] gives an alternative formula for the partial Fréchet derivative of a standard matrix function:

$$\mathsf{D}_{\boldsymbol{X}_{i}}f\left[\boldsymbol{\vec{X}}\right]\left(\boldsymbol{\vec{E}}\right) = \left[\varphi_{i}\left(\bar{\lambda}_{k},\bar{\lambda}_{l}\right)\right]_{kl}\odot\boldsymbol{E}_{i}, \quad \forall \,\boldsymbol{\vec{X}}\in\mathbb{S}^{n} \text{ and } \boldsymbol{\vec{E}}=\left(\boldsymbol{E}_{1},\ldots,\boldsymbol{E}_{n}\right)\in\left(\mathbb{M}^{\mathrm{sa}}\right)^{n},\tag{5}$$

where the $\{X_i\}_{i=1}^n$ are simultaneously diagonalised with λ_{ik} being the k-th eigenvalue of X_i ; $\bar{\lambda}_k \triangleq (\lambda_{1k}, \ldots, \lambda_{ik}, \ldots, \lambda_{nk})$; and \odot denotes the Hadamard product.

3. MATRIX FUNCTIONAL INEQUALITIES

The main results in this section include various matrix functional inequalities for matrix-valued processes.

We first present the definition of the matrix Φ -entropies for random matrices from Chen and Tropp [62], and provide the notation for the Dirichlet forms of matrix-valued functions. Then, we derive the matrix *Poincaré inequalities* for the general multivariate matrix-valued function $\boldsymbol{f} : (\mathbb{M}_{d_1}^{sa})^n \to \mathbb{M}_{d_2}^{sa}$ (Theorem 2), multivariate standard matrix functions (Corollary 3) in Section 3.1. We then extend the matrix *Poincaré inequality* to Gaussian distribution (called matrix Gaussian Poincaré inequality, Theorem 4). These results rely on the matrix Efron-Stein inequality, which was first proven in our previous work [63, Theorem 5.1].

Section 3.2 presents the results on Sobolev inequalities for matrix Φ -entropies. The matrix Φ -Sobolev inequality of symmetric Bernoulli random variables and that of Gaussian random variables are in Theorem 6 and Theorem 7, respectively. The matrix logarithmic Φ -Sobolev inequalities of symmetric Bernoulli random variables are given in Corollaries 8 and 9.

Throughout this section, let $\vec{X} \triangleq (X_1, \ldots, X_n)$ be a series of independent random variables taking values in some Polish space and let $\vec{Z} \triangleq f(\vec{X}) \in \mathbb{M}_d^{\text{sa}}$ be a random matrix such that $\|\mathbb{E}Z^2\|_{\infty} < \infty$. Let X'_i be an independent copy of X_i , for $1 \leq i \leq n$, and denote by $\widetilde{X}^{(i)} \triangleq (X_1, \ldots, X_{i-1}, X'_i, X_{i+1}, \ldots, X_n)$, i.e. replacing the *i*-th component of \vec{X} by the independent copy X'_i . Let $X_{-i} \triangleq (X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_n)$, i.e. replacing the *i*-th component of \vec{X} by the independent copy X'_i . Let $X_{-i} \triangleq (X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_n)$ and $\mathbb{E}_i[\cdot] \triangleq \mathbb{E}[\cdot |X_{-i}]$, i.e. expectation with respect to the *i*-th variable. Finally, denote by $Z'_i \triangleq f(\widetilde{X}^{(i)})$ for every $i = 1, \ldots, n$.

For a convex function $\Phi : \mathbb{R} \to \mathbb{R}$ such that $\mathbb{E} \| \mathbf{Z} \|_{\infty} < \infty$ and $\mathbb{E} \| \Phi(\mathbf{Z}) \|_{\infty} < \infty$, The matrix Φ -entropy $H_{\Phi}(\mathbf{Z})$ is defined as

$$H_{\Phi}(\boldsymbol{Z}) \triangleq \overline{\operatorname{tr}} \left[\mathbb{E} \Phi(\boldsymbol{Z}) - \Phi(\mathbb{E} \boldsymbol{Z}) \right]$$

The (matrix-valued) *local influence* is defined as

$$\mathcal{I}_i(\boldsymbol{f}|\boldsymbol{X}_{-i}) \triangleq rac{1}{2} \mathbb{E}\left[\left(\boldsymbol{f}(ec{\boldsymbol{X}}) - \boldsymbol{f}\left(\widetilde{\boldsymbol{X}}^{(i)}
ight)
ight)^2
ight],$$

for every $i \in 1, ..., n$. This quantity characterises the local fluctuation of the *i*-th position on average. The matrix-valued and real-valued *total influence* of the function f are defined as

$$\mathcal{E}(\mathbf{f}) \triangleq \sum_{i=1}^{n} \mathbb{E}\left[\mathcal{I}_{i}(\mathbf{f}|\mathbf{X}_{-i})\right], \text{ and } \mathcal{E}(\mathbf{f}) \triangleq \overline{\operatorname{tr}} \mathcal{E}(\mathbf{f}).$$
 (6)

Note that we use the notation $\mathcal{E}(f)$ and $\mathcal{E}(Z)$ interchangeably. This quantity is also known as the *Dirichlet* form or energy functional in Markov semigroup theory (see e.g. [12] and [42]). The total influence $\mathcal{E}(Z)$ has the following equivalent expressions (Lemma 11):

$$\boldsymbol{\mathcal{E}}(\boldsymbol{Z}) = \frac{1}{2} \sum_{i=1}^{n} \mathbb{E}\left[\left(\boldsymbol{Z} - \boldsymbol{Z}_{i}^{\prime} \right)^{2} \right] = \sum_{i=1}^{n} \mathbb{E}\left[\left(\boldsymbol{Z} - \mathbb{E}_{i} \boldsymbol{Z} \right)^{2} \right] = \sum_{i=1}^{n} \mathbb{E}\left[\left(\boldsymbol{Z} - \boldsymbol{Z}_{i}^{\prime} \right)_{+}^{2} \right],$$
(7)

where, for $f(x) = \max\{x, 0\}, (A)_+ = f(A)$ denotes the contribution from its positive eigenvalues.

3.1. The Matrix Poincaré Inequality. We denote the matrix-valued and real-valued variance of a random matrix A (taking values in \mathbb{M}_d^{sa}) by

$$\operatorname{Var}(A) \triangleq \left[\mathbb{E} \left(A - \mathbb{E} A \right)^2 \right] = \left[\mathbb{E} A^2 - \left(\mathbb{E} A \right)^2 \right], \text{ and } \operatorname{Var}(A) \triangleq \overline{\operatorname{tr}} \operatorname{Var}(A).$$

In the following, we recall the result from our previous work [63] and Eq. (7) to present a matrix Efron-Stein inequality, which plays a major role in the matrix Poincaré inequality.

Theorem 1 (Matrix Efron-Stein Inequality [63, Theorem 5.1]). With the prevailing assumptions, we have

$$\operatorname{Var}(\boldsymbol{Z}) \preceq \boldsymbol{\mathcal{E}}(\boldsymbol{Z}) = \sum_{i=1}^{n} \mathbb{E}\left[\left(\boldsymbol{Z} - \boldsymbol{Z}_{i}^{\prime} \right)_{+}^{2} \right].$$
(8)

Remark 3.1. In addition to Eq. (7), the quantity $\mathcal{E}(\mathbf{Z})$ also has the following minimum representation:

$$\boldsymbol{\mathcal{E}}(\boldsymbol{Z}) = \sum_{i=1}^{n} \min_{\boldsymbol{Z}_{i}} \mathbb{E}\left[(\boldsymbol{Z} - \boldsymbol{Z}_{i})^{2} \right], \tag{9}$$

where the minimum is taken over the class of all (\mathbf{X}_{-i}) -measurable random matrix \mathbf{Z}_i such that $\|\mathbb{E}\mathbf{Z}_i^2\|_{\infty} < \infty$. The identity follows from the fact that $\operatorname{Var}(\mathbf{A}) = \min_{\mathbf{u} \in \mathbb{M}_d^{sa}} \mathbb{E}\left[(\mathbf{A} - \mathbf{u})^2\right]$, for any random matrix \mathbf{A} taking values in \mathbb{M}_d^{sa} . Therefore, for every $i = 1, \ldots, n$, $\operatorname{Var}^{(i)}(\mathbf{Z}) = \min_{\mathbf{u}} \mathbb{E}_i\left[(\mathbf{Z} - \mathbf{u})^2\right]$, where the infimum is taken over the class of all (\mathbf{X}_{-i}) -measurable and square-integrable matrices \mathbf{u} . Note that the minimum is attained as $\mathbf{u} = \mathbb{E}_i \mathbf{Z}$.

The matrix Efron-Stein inequality can be used to prove a matrix version of the Poincaré inequality.

Theorem 2 (Matrix Poincaré Inequality). Let $\vec{X} = (X_1, \ldots, X_n) \in (\mathbb{M}_{d_1}^{sa})^n$ be an n-tuple independent random matrix taking values in the interval [0, I] (under the Löwner partial ordering) and let $f : (\mathbb{M}_{d_1}^{sa}([0,1]))^n \to \mathbb{M}_{d_2}^{sa}$ be a separately convex function² with finite partial Fréchet derivatives. Then $f(\vec{X}) = f(X_1, \ldots, X_n)$ satisfies

$$\operatorname{Var}\left(\boldsymbol{f}\left(\boldsymbol{\vec{X}}\right)\right) \leq \sum_{i=1}^{n} \mathbb{E}\left[\left\|\mathsf{D}_{\boldsymbol{X}_{i}}\boldsymbol{f}\left[\boldsymbol{\vec{X}}\right]\right\|_{2}^{2}\right],\tag{10}$$

where $\|\mathsf{D}_{\mathbf{X}_i} \mathbf{f}[\mathbf{X}]\|_2$ is the norm of the Fréchet derivative defined in Eq. (2).

Moreover, if f is separately monotone decreasing, then Eq. (10) can be strengthened to

$$\operatorname{Var}\left(\boldsymbol{f}\left(\boldsymbol{\vec{X}}\right)\right) \preceq_{\mathrm{U}} \sum_{i=1}^{n} \mathbb{E}\left[\left(\mathsf{D}_{\boldsymbol{X}_{i}}\boldsymbol{f}\left[\boldsymbol{\vec{X}}\right](\boldsymbol{I})\right)^{2}\right].$$
(11)

Proof. Recall $\mathbf{Z} \equiv \mathbf{f}(\vec{\mathbf{X}})$ and $\mathbf{Z}_i \equiv \mathbf{f}(\widetilde{\mathbf{X}}^{(i)}) = \mathbf{f}(\mathbf{X}_1, \dots, \mathbf{X}_{i-1}, \mathbf{X}'_i, \mathbf{X}_{i+1}, \dots, \mathbf{X}_n)$, where \mathbf{X}'_i is an identical copy of \mathbf{X}_i . The proof follows from the matrix Efron-Stein inequality (Theorem 1):

$$\operatorname{Var}\left(\boldsymbol{f}\left(\boldsymbol{\vec{X}}\right)\right) = \operatorname{Var}\left(\boldsymbol{Z}\right) \preceq \sum_{i=1}^{n} \mathbb{E}\left(\boldsymbol{Z} - \boldsymbol{Z}_{i}\right)_{+}^{2}.$$
(12)

It then suffices to bound each term $\mathbb{E} \left(\boldsymbol{Z} - \boldsymbol{Z}_i \right)_+^2$ on the right-hand side above:

$$(\boldsymbol{Z} - \boldsymbol{Z}_{i})_{+}^{2} = \left(\boldsymbol{f}\left(\boldsymbol{\vec{X}}\right) - \boldsymbol{f}\left(\boldsymbol{\widetilde{X}}^{(i)}\right)\right)_{+}^{2} \leq_{\mathrm{U}} \left(\mathsf{D}_{\boldsymbol{X}_{i}}\boldsymbol{f}\left[\boldsymbol{\vec{X}}\right]\left(\boldsymbol{X}_{i} - \boldsymbol{X}_{i}^{\prime}\right)\right)_{+}^{2}$$
(13)

$$\preceq_{\mathrm{U}} \left(\mathsf{D}_{\boldsymbol{X}_{i}} \boldsymbol{f} \left[\boldsymbol{\vec{X}} \right] (\boldsymbol{I}) \right)^{2}, \qquad (14)$$

where the first inequality follows from the separate convexity (see e.g. [64, Chapter 3]):

$$\boldsymbol{f}\left(\vec{\boldsymbol{X}}\right) - \boldsymbol{f}\left(\widetilde{\boldsymbol{X}}^{(i)}\right) \preceq \mathsf{D}_{\boldsymbol{X}_{i}}\boldsymbol{f}\left[\vec{\boldsymbol{X}}\right]\left(\boldsymbol{X}_{i} - \boldsymbol{X}_{i}^{\prime}\right),\tag{15}$$

as well as the fact that $A_+ \leq B_+$ implies $A_+^2 \leq_U B_+^2$. The second line is due to the separately monotone decreasing property: $\mathsf{D}_{\mathbf{X}_i} f[\vec{\mathbf{X}}](\mathbf{A}) \leq 0$ for all $\mathbf{A} \succeq 0$. Hence $(\mathsf{D}_{\mathbf{X}_i} f[\vec{\mathbf{X}}](\mathbf{X}_i - \mathbf{X}'_i))_+ \leq -\mathsf{D}_{\mathbf{X}_i} f[\vec{\mathbf{X}}](\mathbf{I})$, which proving Eq. (11).

If f is not separately monotone decreasing, Eq. (14) does not generally hold. To show Eq. (10), we take the normalised trace on both sides of Eq. (13):

$$\begin{split} \overline{\operatorname{tr}} \left(\boldsymbol{Z} - \boldsymbol{Z}_{i} \right)_{+}^{2} &\leq \overline{\operatorname{tr}} \left(\mathsf{D}_{\boldsymbol{X}_{i}} \boldsymbol{f} \left[\boldsymbol{\vec{X}} \right] \left(\boldsymbol{X}_{i} - \boldsymbol{X}_{i}' \right) \right)_{+}^{2} \leq \overline{\operatorname{tr}} \left| \mathsf{D}_{\boldsymbol{X}_{i}} \boldsymbol{f} \left[\boldsymbol{\vec{X}} \right] \left(\boldsymbol{X}_{i} - \boldsymbol{X}_{i}' \right) \right|^{2} \\ &= \frac{1}{d_{2}} \left\| \mathsf{D}_{\boldsymbol{X}_{i}} \boldsymbol{f} \left[\boldsymbol{\vec{X}} \right] \left(\boldsymbol{X}_{i} - \boldsymbol{X}_{i}' \right) \right\|_{2}^{2} \leq \frac{1}{d_{2}} \left\| \mathsf{D}_{\boldsymbol{X}_{i}} \boldsymbol{f} \left[\boldsymbol{\vec{X}} \right] \right\|_{2}^{2} \cdot \left\| \boldsymbol{X}_{i} - \boldsymbol{X}_{i}' \right\|_{2}^{2} \\ &\leq \frac{1}{d_{2}} \left\| \mathsf{D}_{\boldsymbol{X}_{i}} \boldsymbol{f} \left[\boldsymbol{\vec{X}} \right] \right\|_{2}^{2} \cdot \left\| \boldsymbol{I} \right\|_{2}^{2} = \left\| \mathsf{D}_{\boldsymbol{X}_{i}} \boldsymbol{f} \left[\boldsymbol{\vec{X}} \right] \right\|_{2}^{2}. \end{split}$$

The equality in the second line follows from the definition of Schatten 2-norm. The inequality in the second line follows directly from the norm of Fréchet derivatives, i.e. $\|\mathsf{D}f[A](B)\|_2 \leq \|\mathsf{D}f[A]\|_2 \cdot \|B\|_2$. Finally, we use the assumption $\mathbf{0} \leq \mathbf{X}_i, \mathbf{X}'_i \leq \mathbf{I}$ and $\|\mathbf{I}\|_2 = \sqrt{d_2}$ in the third line to complete the proof.

$$t\boldsymbol{f}(\boldsymbol{Y}) + (1-t)\boldsymbol{f}\left(\widetilde{\boldsymbol{Y}}^{(i)}\right) \preceq \boldsymbol{f}\left(t\widetilde{\boldsymbol{Y}} + (1-t)\widetilde{\boldsymbol{Y}}^{(i)}\right)$$

for $\vec{Y} = (Y_1, \dots, Y_n) \in (\mathbb{M}_d^{sa})^n$, and $\widetilde{Y}^{(i)} = (Y_1, \dots, Y_{i-1}, Y'_i, Y_{i+1}, \dots, Y_n) \in (\mathbb{M}_d^{sa})^n$. The separate monotonicity is defined similarly.

²Note that \boldsymbol{f} here is a multivariate super-operator. The separate convexity means that: for $0 \le t \le 1$,

Note that Theorem 2 generalises the classical Poincaré inequality (e.g. [48, Theorem 3.17]):

$$\operatorname{Var}(f(X)) \leq \mathbb{E}\left[\|\nabla f(X)\|^2 \right],$$

where $X \triangleq (X_1, \ldots, X_n)$ denotes an independent random vector and each element takes values in the interval [0, 1].

Theorem 2 considers the matrix Poincaré inequality for general matrix functions $\boldsymbol{f} : (\mathbb{M}_d^{\mathrm{sa}})^n \to \mathbb{M}_d^{\mathrm{sa}}$, while in Corollary 3 below, we impose additional pairwise commutative criteria on $\boldsymbol{X} = (\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n)$; namely, $[\boldsymbol{X}_i, \boldsymbol{X}_j] = \boldsymbol{0}$ almost surely for $i \neq j \in [n]$. We establish the following Matrix Poincaré inequality for multivariate standard matrix functions (see Eq. (3)).

Corollary 3 (Matrix Poincaré Inequality for Multivariate Standard Matrix Functions). Let $\vec{X} = (X_1, \ldots, X_n)$ be an n-tuple independent random matrix taking values in \mathbb{S}^n_d with joint spectrum in $[0,1]^n$. Let f: $([0,1])^n \to \mathbb{R}$ be a multivariate standard matrix function that is separately operator convex and has finite partial Fréchet derivatives. Then, $f(\vec{X}) = f(X_1, \ldots, X_n)$ satisfies

$$\mathbf{Var}\left(f\left(\vec{\boldsymbol{X}}\right)\right) \preceq_{\mathrm{U}} \sum_{i=1}^{n} \mathbb{E}\left[\left(\left[\varphi_{i}\left(\bar{\lambda}_{k}, \bar{\lambda}_{\ell}\right)\right]_{k\ell} \odot \boldsymbol{I}\right)^{2}\right],$$

where φ_i is the divided difference of f defined in Eq. (4), and $\bar{\lambda}_k \triangleq (\lambda_{1k}, \ldots, \lambda_{ik}, \ldots, \lambda_{nk})$ with λ_{ik} being the *i*-th eigenvalue of \mathbf{X}_k .

Proof. Following the same argument in the proof of Theorem 2, we have

$$\mathsf{D}_{\boldsymbol{X}_{i}}f[\boldsymbol{\vec{X}}]\left(\boldsymbol{X}_{i}-\boldsymbol{X}_{i}'\right)=\left[\varphi_{i}\left(\bar{\lambda}_{k},\bar{\lambda}_{\ell}\right)\right]_{k\ell}\odot\left(\boldsymbol{X}_{i}-\boldsymbol{X}_{i}'\right)\preceq\left[\varphi_{i}\left(\bar{\lambda}_{k},\bar{\lambda}_{\ell}\right)\right]_{k\ell}\odot\boldsymbol{I},$$

where the equality follows from the multivariate version of Daleckiĭ and Kreĭn formula (5), and the inequality is a direct consequence of Schur's product theorem: $\mathbf{A} \odot \mathbf{B} \leq \mathbf{A} \odot \mathbf{I} \cdot \|\mathbf{B}\|_{\infty}$ [65].

The matrix Efron-Stein inequality is used in Theorem 2 to prove the matrix Poincaré inequality. Next we will show that the matrix Efron-Stein inequality can be also applied to establish an upper bound, known as the *Gaussian Poincaré inequality*, for a Fréchet differentiable matrix-valued function of *Gaussian Unitary Ensembles* $(GUE)^3$.

Theorem 4 (Matrix Poincaré Inequality for GUE). Let X_1, \ldots, X_n be independent random matrices⁴ from the Gaussian Unitary Ensemble and let $\boldsymbol{f} : (\mathbb{M}_{d_1}^{\mathrm{sa}})^n \to \mathbb{M}_{d_2}^{\mathrm{sa}}$ be any twice Fréchet differentiable function. Then $\boldsymbol{f}(\vec{X})$ satisfies

$$\operatorname{Var}\left(\boldsymbol{f}\left(\boldsymbol{\vec{X}}\right)\right) \leq \sum_{i=1}^{n} \mathbb{E}\left[\left\|\mathsf{D}_{\boldsymbol{X}_{i}}\boldsymbol{f}\left[\boldsymbol{\vec{X}}\right]\right\|_{2}^{2}\right].$$

Proof. Borrowing the idea from [15] (see also [48, Theorem 3.20]) to prove this theorem. We first assume $\sum_{i=1}^{n} \mathbb{E} \| \mathsf{D}_{\mathbf{X}_{i}} \mathbf{f}[\vec{\mathbf{X}}] \|_{2}^{2} < \infty$; otherwise the inequality trivially holds. Then, it suffices to establish this theorem for n = 1:

$$\operatorname{Var}\left(\boldsymbol{f}(\boldsymbol{X})\right) \leq \mathbb{E}\left[\left\|\mathsf{D}\boldsymbol{f}[\boldsymbol{X}]\right\|_{2}^{2}\right],\tag{16}$$

and it can be easily extended to every $n \in \mathbb{N}$ by applying the matrix Efron-Stein inequality, Theorem 1.

Now, for every $j \in [m] \triangleq \{1, \ldots, m\}$, denote by W_j , W'_j the $d_1 \times d_1$ matrices whose entries are sampled from independent Rademacher random variables (i.e. uniformly $\{\pm 1\}$ -valued random variables). Let

$$\mathbf{Y}_{j} = \frac{\left(\mathbf{W}_{j} + \mathbf{i} \cdot \mathbf{W}_{j}^{\prime}\right) + \left(\mathbf{W}_{j} + \mathbf{i} \cdot \mathbf{W}_{j}^{\prime}\right)^{\dagger}}{2}.$$

³The Gaussian Unitary Ensembles are a family of random Hermitian matrices whose upper-triangular entries are independently and identically distributed (i.i.d.) complex standard Gaussian random variables, while the diagonal entries are i.i.d. real standard Gaussian random variables, see e.g. $[66, \S 2.6]$

⁴We consider "entry-wise" independence here.

Denote by $\epsilon_1, \ldots, \epsilon_m$ a series of independent Rademacher random variables, and define $S_m \triangleq \frac{1}{\sqrt{m}} \sum_{j=1}^m \epsilon_j Y_j$. Then, for every $j \in [m]$,

$$\operatorname{Var}^{(j)}\left(\boldsymbol{f}(\boldsymbol{S}_{m})\right) = \frac{1}{4} \operatorname{\overline{tr}} \mathbb{E}_{\boldsymbol{Y}_{j}}\left[\left(\boldsymbol{f}\left(\boldsymbol{S}_{m} + \frac{1-\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right) - \boldsymbol{f}\left(\boldsymbol{S}_{m} - \frac{1+\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right)\right)^{2}\right].$$

We invoke the matrix Efron-Stein inequality to obtain

$$\operatorname{Var}\left(\boldsymbol{f}(\boldsymbol{S}_{m})\right) \leq \frac{1}{4} \sum_{j=1}^{m} \operatorname{\overline{tr}} \mathbb{E}\left[\left(\boldsymbol{f}\left(\boldsymbol{S}_{m} + \frac{1-\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right) - \boldsymbol{f}\left(\boldsymbol{S}_{m} - \frac{1+\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right)\right)^{2}\right],\tag{17}$$

and then use Taylor's expansion to further bound the right-hand side of Eq. (17). For every $i \in [n]$ and some constants $0 \le \alpha, \beta \le 1$, it follows almost surely that

$$\begin{split} \boldsymbol{f}\left(\boldsymbol{S}_{m} + \frac{1-\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right) &= \boldsymbol{f}(\boldsymbol{S}_{m}) + \mathsf{D}\boldsymbol{f}[\boldsymbol{S}_{m}]\left(\frac{1-\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right) + \mathcal{R}_{2}\left(\boldsymbol{S}_{m}, \frac{1-\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right);\\ \boldsymbol{f}\left(\boldsymbol{S}_{m} - \frac{1+\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right) &= \boldsymbol{f}(\boldsymbol{S}_{m}) + \mathsf{D}\boldsymbol{f}[\boldsymbol{S}_{m}]\left(-\frac{1+\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right) + \mathcal{R}_{2}\left(\boldsymbol{S}_{m}, -\frac{1+\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right),\\ \boldsymbol{f}\left(\boldsymbol{S}_{m} - \frac{1+\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right) &= \boldsymbol{f}(\boldsymbol{S}_{m}) + \mathsf{D}\boldsymbol{f}[\boldsymbol{S}_{m}]\left(-\frac{1+\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right) + \mathcal{R}_{2}\left(\boldsymbol{S}_{m}, -\frac{1+\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right), \end{split}$$

where $\mathcal{R}_l : \mathbb{M}_{d_1} \times \mathbb{M}_{d_1} \to \mathbb{M}_{d_2}$ is the remainder term of the Taylor series:

$$\mathcal{R}_{l}(\boldsymbol{X}, \boldsymbol{E}) \triangleq \sum_{k=l}^{\infty} \frac{1}{k!} \mathsf{D}^{k} \boldsymbol{f}[\boldsymbol{X}] (\underbrace{\boldsymbol{E}, \dots, \boldsymbol{E}}_{k}) = o\left(|\boldsymbol{E}|^{l}\right)$$

Therefore,

$$\boldsymbol{f}\left(\boldsymbol{S}_{m}+\frac{1-\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right)-\boldsymbol{f}\left(\boldsymbol{S}_{m}-\frac{1+\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right) \leq \frac{2}{\sqrt{m}}\mathsf{D}\boldsymbol{f}[\boldsymbol{S}_{m}]\left(\boldsymbol{Y}_{j}\right)+o\left(\frac{1}{m}\right),$$

and

$$\frac{1}{4}\sum_{j=1}^{m}\overline{\operatorname{tr}} \mathbb{E}\left[\left(\boldsymbol{f}\left(\boldsymbol{S}_{m}+\frac{1-\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right)-\boldsymbol{f}\left(\boldsymbol{S}_{m}-\frac{1+\epsilon_{j}}{\sqrt{m}}\boldsymbol{Y}_{j}\right)\right)^{2}\right] \leq \left\|\mathsf{D}\boldsymbol{f}[\boldsymbol{S}_{m}]\right\|_{2}^{2}+o\left(\frac{1}{\sqrt{m}}\right).$$

Let m go to infinity, we have

$$\lim_{m \to \infty} \frac{1}{4} \sum_{i=1}^{m} \overline{\operatorname{tr}} \mathbb{E} \left[\left(\boldsymbol{f} \left(\boldsymbol{S}_{m} + \frac{1 - \epsilon_{j}}{\sqrt{m}} \boldsymbol{Y}_{j} \right) - \boldsymbol{f} \left(\boldsymbol{S}_{m} - \frac{1 + \epsilon_{j}}{\sqrt{m}} \boldsymbol{Y}_{j} \right) \right)^{2} \right] \leq \mathbb{E} \left[\left\| \mathsf{D} \boldsymbol{f} [\boldsymbol{X}] \right\|_{2}^{2} \right],$$
(18)

where, by the central limit theorem (see Lemma 12), S_m converges in distribution to a random matrix \boldsymbol{X} in GUE. Thus Var $(\boldsymbol{f}(\boldsymbol{S}_m))$ converges to Var $(\boldsymbol{f}(\boldsymbol{X}))$.

Finally, the subadditivity of the variance and Eq. (16) lead to

$$\operatorname{Var}\left(\boldsymbol{f}\left(\boldsymbol{\vec{X}}\right)\right) \leq \sum_{i=1}^{n} \mathbb{E}\left[\operatorname{Var}^{(i)}\left(\boldsymbol{f}\left(\boldsymbol{\vec{X}}\right)\right)\right] \leq \sum_{i=1}^{n} \mathbb{E}\left[\mathbb{E}_{i}\left[\left\|\mathsf{D}_{\boldsymbol{X}_{i}}\boldsymbol{f}\left[\boldsymbol{\vec{X}}\right]\right\|_{2}^{2}\right]\right] = \sum_{i=1}^{n} \mathbb{E}\left[\left\|\mathsf{D}_{\boldsymbol{X}_{i}}\boldsymbol{f}\left[\boldsymbol{\vec{X}}\right]\right\|_{2}^{2}\right],$$

ch completes the proof.

which completes the proof.

3.2. Matrix Φ -Sobolev Inequalities. In this section, we consider matrix-valued functions defined on Boolean hypercubes: $f: \{0,1\} \to \mathbb{M}_d^{\text{sa}}$ and establish matrix Φ -Sobolev inequalities. The main ingredient to prove this inequality comes from Fourier analysis and the hypercontractive inequality for matrix-valued functions.

Ben-Aroya et al. [19] generalised Bonami and Beckner's results by considering matrix-valued functions $f: \{0,1\} \to \mathbb{M}_d$. Similarly, Fourier analysis can be naturally extended into the matrix setting; that is, the Fourier transform \widehat{f} of the matrix-valued function f can be expressed as

$$\begin{cases} \widehat{\boldsymbol{f}}(S) = \frac{1}{2^n} \sum_{x \in \{0,1\}^n} \boldsymbol{f}(x) u_S(x); \\ \boldsymbol{f}(x) = \sum_{S \subseteq \{1,\dots,n\}} \widehat{\boldsymbol{f}}(S) u_S(x), \end{cases}$$

where $u_S(x) \triangleq \prod_{i \in S} (-1)^{x_i}$. Therefore, the classical hypercontractive inequality [4, 5] can be extended to matrix-valued functions.

Theorem 5 (Matrix Bonami-Gross-Beckner Inequality [19]). For every $\boldsymbol{f}: \{0,1\}^n \to \mathbb{M}_d$ and $1 \leq p \leq 2$,

$$\left(\sum_{S\subseteq[n]} (p-1)^{|S|} \left\| \widehat{f}(S) \right\|_p^2 \right)^{1/2} \le \left(\frac{1}{2^n} \sum_{x \in \{0,1\}^n} \left\| f(x) \right\|_p^p \right)^{1/p}$$

With Theorem 5, we can prove a matrix Φ -Sobolev inequality for matrix-valued functions defined on symmetric Bernoulli random variables.

Theorem 6 (Matrix Φ -Sobolev Inequalities for Symmetric Bernoulli Random Variables). Let X be uniformly distributed over $\mathcal{X} \equiv \{0,1\}^n$ (an n-dimensional binary hypercube) and $\mathbf{f} : \mathcal{X} \to \mathbb{M}_d^+$ be an arbitrary matrix-valued function. Then for all $p \in (1,2)$, and $\Phi(u) = u^{2/p}$,

$$H_{\Phi}(\boldsymbol{f}^p) \le (2-p)\mathcal{E}(\boldsymbol{f}) \cdot d^{1-2/p} + \operatorname{tr} \mathbb{E}[\boldsymbol{f}^2] \cdot (1-d^{1-2/p}).$$
(19)

Proof. Starting from the left-hand side of Eq. (19), the definition of the matrix Φ -entropy functional gives

$$H_{\Phi}(\boldsymbol{f}^{p}) = \overline{\operatorname{tr}} \mathbb{E} \left[\boldsymbol{f}^{2} \right] - \overline{\operatorname{tr}} \left[(\mathbb{E} \boldsymbol{f}^{p})^{2/p} \right] \leq \overline{\operatorname{tr}} \mathbb{E} \left[\boldsymbol{f}^{2} \right] - \left(\overline{\operatorname{tr}} \mathbb{E} \boldsymbol{f}^{p} \right)^{2/p}$$
$$= \overline{\operatorname{tr}} \mathbb{E} \left[\boldsymbol{f}^{2} \right] - \left(\mathbb{E} \left\| \boldsymbol{f} \right\|_{p}^{p} \right)^{2/p} \cdot d^{-2/p},$$
(20)

where we apply the convexity of $\overline{\text{tr}}$, and recall that $(\cdot)^{2/p}$ is a convex function for $1 \le p \le 2$.

We then apply Theorem 5 to Eq. (20) to obtain

$$H_{\Phi}(\boldsymbol{f}^{p}) \leq \overline{\operatorname{tr}} \mathbb{E} \left[\boldsymbol{f}^{2} \right] - \left(\sum_{S \subseteq [n]} (p-1)^{|S|} \left\| \widehat{\boldsymbol{f}}(S) \right\|_{p}^{2} \right) \cdot d^{-2/p}$$

$$\leq \overline{\operatorname{tr}} \mathbb{E} \left[\boldsymbol{f}^{2} \right] - \left(\sum_{S \subseteq [n]} (p-1)^{|S|} \overline{\operatorname{tr}} \left[\widehat{\boldsymbol{f}}(S)^{2} \right] \right) \cdot d^{1-2/p}$$

$$= \overline{\operatorname{tr}} \left[\sum_{S \subseteq [n]} \widehat{\boldsymbol{f}}(S)^{2} \right] - \left(\sum_{S \subseteq [n]} (p-1)^{|S|} \overline{\operatorname{tr}} \left[\widehat{\boldsymbol{f}}(S)^{2} \right] \right) \cdot d^{1-2/p}$$

$$= \overline{\operatorname{tr}} \left[\sum_{S \subseteq [n]} \left(1 - (p-1)^{|S|} d^{1-2/p} \right) \widehat{\boldsymbol{f}}(S)^{2} \right], \qquad (21)$$

where the second inequality is because the Schatten p-norm is non-increasing, and we apply Parseval's identity (Lemma 13 in Appendix A) in the third line.

From the elementary analysis, it can be verified that, for all $S \subseteq [n]$ and $1 \leq p \leq 2$, $1 - (p-1)^{|S|} \leq (2-p)|S|$. Therefore, it follows that

$$1 - (p-1)^{|S|} d^{1-2/p} \le (2-p)|S| d^{1-2/p} + (1 - d^{1-2/p}).$$

Finally, given $\sum_{S \subseteq [n]} \overline{\operatorname{tr}} \left[|S| \widehat{f}(S)^2 \right] = \mathcal{E}(f)$ (see Lemma 14 in Appendix A), Eq. (21) can be further deduced as

$$H_{\Phi}(\boldsymbol{f}^{p}) \leq \overline{\operatorname{tr}} \left[\sum_{S \subseteq [n]} \left(1 - (p-1)^{|S|} d^{1-2/p} \right) \widehat{\boldsymbol{f}}(S)^{2} \right]$$

$$\leq \overline{\operatorname{tr}} \left[\sum_{S \subseteq [n]} \left((2-p) |S| d^{1-2/p} + (1-d^{1-2/p}) \right) \widehat{\boldsymbol{f}}(S)^{2} \right]$$

$$= (2-p) \mathcal{E}(\boldsymbol{f}) \cdot d^{1-2/p} + \overline{\operatorname{tr}} \mathbb{E}[\boldsymbol{f}^{2}] \cdot (1-d^{1-2/p}),$$

which completes our claim.

Theorem 7 (Matrix Φ -Sobolev Inequalities for Gaussian Distributions). Let $X = (X_1, \ldots, X_n)$ be a vector of n independent standard Gaussian random variables taking values in $\mathcal{X} \equiv \mathbb{R}^n$, and let $f : \mathcal{X} \rightarrow \mathcal{X}$ \mathbb{M}_d^+ be an arbitrary matrix-valued function. Then for all $p \in (1,2)$, and $\Phi(u) = u^{2/p}$,

$$H_{\Phi}(\boldsymbol{f}^{p}) \le (2-p) \sum_{i=1}^{n} \mathbb{E}\left[\left\| \mathsf{D}_{X_{i}} \boldsymbol{f}[X] \right\|_{2}^{2} \right] \cdot d^{1-2/p} + \overline{\operatorname{tr}} \mathbb{E}[\boldsymbol{f}^{2}] \cdot (1-d^{1-2/p}).$$
(22)

Proof. The proof parallels the approach in Theorem 4. Recall from Eq. (18) and let $Y_i \equiv 1$:

$$\mathcal{E}^{(i)}(\boldsymbol{f}) = \lim_{m \to \infty} \frac{1}{4} \sum_{i=1}^{m} \overline{\operatorname{tr}} \mathbb{E}_{i} \left[\left(\boldsymbol{f} \left(S_{m} + \frac{1 - \epsilon_{i}}{\sqrt{m}} \right) - \boldsymbol{f} \left(S_{m} - \frac{1 + \epsilon_{i}}{\sqrt{m}} \right) \right)^{2} \right] = \mathbb{E}_{i} \left[\left\| \mathsf{D}_{X_{i}} \boldsymbol{f}[X] \right\|_{2}^{2} \right].$$
and Theorem (6) yield Eq. (7) and the statement follows.

This and Theorem (6) yield Eq. (7) and the statement follows.

The logarithmic Sobolev inequality for matrix-valued functions immediately follows from Theorems 6 and 7. Subsequently, we denote by

$$\operatorname{Ent}(\boldsymbol{Z}) := H_{\Phi}(\boldsymbol{Z}), \quad \text{when } \Phi(u) = u \log u.$$
(23)

Corollary 8 (Matrix Log-Sobolev Inequalities for Symmetric Bernoulli Random Variables). Let f: $\{0,1\}^n \to \mathbb{M}_d^+$ be an arbitrary matrix-valued function defined on the n-dimensional binary hypercube and assume that X is uniformly distributed over $\{0,1\}^n$. Then

$$\operatorname{Ent}(\boldsymbol{f}^2) \leq 2\mathcal{E}(\boldsymbol{f}) + \log(d) \cdot \operatorname{\overline{tr}} \mathbb{E}\left[\boldsymbol{f}^2\right].$$

Proof. By letting $p \to 2$, the left-hand side of Eq. (19) becomes

$$\lim_{p \to 2^{-}} \frac{H_{\Phi}(\boldsymbol{f}^p)}{2-p} = \lim_{p \to 2^{-}} \frac{\overline{\operatorname{tr}}\left[\mathbb{E}\left[\boldsymbol{f}(X)^2\right] - \left(\mathbb{E}\left[\boldsymbol{f}(X)^p\right]^{2/p}\right)\right]}{2-p} = \frac{\operatorname{Ent}(\boldsymbol{f}^2)}{2},$$

where the last identity follows from Lemma 15. Similarly, the right-hand side gives

$$\lim_{p \to 2^{-}} \frac{(2-p)\mathcal{E}(\boldsymbol{f}) \cdot d^{1-2/p} + \overline{\operatorname{tr}} \mathbb{E}\left[\boldsymbol{f}^{2}\right] \cdot (1-d^{1-2/p})}{2-p} = \mathcal{E}(\boldsymbol{f}) + \frac{\log(d)}{2} \cdot \overline{\operatorname{tr}} \mathbb{E}\left[\boldsymbol{f}^{2}\right]$$

as established.

Corollary 9 (Matrix Gaussian Logarithmic Sobolev Inequalities). Assume that X is a vector of independent and identical standard Gaussian random variables on \mathbb{R}^n and let $f: \mathbb{R}^n \to \mathbb{M}_d^+$ be an arbitrary matrix-valued function of X. Then,

$$\operatorname{Ent}(\boldsymbol{f}^2) \leq 2\sum_{i=1}^n \mathbb{E}\left[\left\|\mathsf{D}_{X_i}\boldsymbol{f}[X]\right\|_2^2\right] + \log(d) \cdot \operatorname{tr} \mathbb{E}\left[\boldsymbol{f}^2\right].$$

Remark 3.2. Denoted by LS(C, D) (see e.g. [12, Section 5.1]) the set of log-Sobolev inequalities with constants $C > 0, D \ge 0$:

$$\operatorname{Ent}(f^2) \le 2C\mathcal{E}(f) + D\mathbb{E}[f^2].$$

When D = 0, the log-Sobolev inequality is called *tight*; otherwise, it is called *defective*. It is well known that the best constants of the classical log-Sobolev inequalities for symmetric Bernoulli random variables and standard Gaussian random variables are (C, D) = (1, 0) [4, 14]. However, numerical simulation shows that examples (d > 1) exist for matrix-valued functions so that: $\operatorname{Ent}(f^2) > 2\mathcal{E}(f)$. In Corollary 8, we establish the log-Sobolev inequality with constant $(C, D) = (1, \log d)$.

We also emphasize that such *defectiveness* in the quantum case has been proved by a recent paper [67]. Moreover, whether the established constant $(C, D) = (1, \log d)$ is optimal for matrix-valued functions with Bernoulli random variables is still open.

 \diamond

4. Entropic Inequality for Classical-Quantum Ensembles

In this section, we connect the matrix Φ -entropies with quantum information theory and present a functional inequality for the classical-quantum (c-q) ensembles that undergo a special Markov evolution.

We follow the notation in Refs. [53, 17]. Let \mathcal{X} be a sample space. We denote by $\mathcal{P}(\mathcal{X})$ the set of all probability distributions on \mathcal{X} and by $\mathcal{P}_*(\mathcal{X})$ the subset of $\mathcal{P}(\mathcal{X})$ which consists of all strictly positive distributions. The set of all $d \times d$ matrix-valued functions on \mathcal{X} is denoted by $\mathcal{F}(\mathcal{X})$; $\mathcal{F}_*(\mathcal{X})$ and $\mathcal{F}^0_*(\mathcal{X})$ are the subsets of $\mathcal{F}(\mathcal{X})$ consisting of all strictly positive and non-negative functions, respectively.

Any classical discrete channel or Markov kernel with input alphabet \mathcal{X} and output alphabet \mathcal{Y} can be described by a transition probabilities $\{K(y|x) : x \in \mathcal{X}, y \in \mathcal{Y}\}$. For any probability distribution μ defined on the alphabet \mathcal{X} , we denote the channel acting on μ from the right and acting on matrix-valued functions $\mathbf{f} \in \mathcal{F}(\mathcal{Y})$ respectively by

$$\mu K(y) \triangleq \sum_{x \in \mathcal{X}} \mu(x) K(y|x), \quad y \in \mathcal{Y}, \quad \text{and} \quad K \boldsymbol{f}(x) \triangleq \sum_{y \in \mathcal{Y}} K(y|x) \boldsymbol{f}(y), \quad x \in \mathcal{X}.$$
(24)

The set of all classical channels is denoted by $\mathcal{M}(\mathcal{Y}|\mathcal{X})$. If $\mu \otimes K \in \mathcal{P}(\mathcal{X}) \times \mathcal{M}(\mathcal{Y}|\mathcal{X})$ denotes the distribution of a random pair $(X, Y) \in \mathcal{X} \times \mathcal{Y}$ with $P_X = \mu$ and $P_{Y|X} = K$, then

$$K\boldsymbol{f}(x) = \mathbb{E}[\boldsymbol{f}(Y)|X = x]$$
(25)

for any $f \in \mathcal{F}(\mathcal{Y})$ and $x \in \mathcal{X}$. We say that a pair $(\mu, K) \in \mathcal{P}(\mathcal{X}) \times \mathcal{M}(\mathcal{Y}|\mathcal{X})$ is admissible if $\mu \in \mathcal{P}_*(\mathcal{X})$ and $\mu K \in \mathcal{P}_*(\mathcal{Y})$. Hence the backward or adjoint channel $K^* \in \mathcal{M}(\mathcal{X}|\mathcal{Y})$ can be defined by

$$K^*(x|y) = \frac{K(y|x)\mu(x)}{\mu K(y)}, \quad (x,y) \in \mathcal{X} \times \mathcal{Y}.$$
(26)

If $(X, Y) \sim \mu \times K$, it follows that $K^* = P_{X|Y}$ and

$$K^* \boldsymbol{f}(y) = \mathbb{E}[\boldsymbol{f}(X)|Y=y]$$
(27)

for any $\boldsymbol{f} \in \mathfrak{F}(\mathcal{X})$ and $y \in \mathcal{Y}$.

Define the conditional matrix Φ -entropy of Z given Y which takes values in any Polish space can be defined by

$$H_{\Phi}(\boldsymbol{Z}|Y) \triangleq \overline{\operatorname{tr}} \mathbb{E} \left[\Phi(\boldsymbol{Z})|Y \right] - \overline{\operatorname{tr}} \left[\Phi \left(\mathbb{E} \left[\boldsymbol{Z}|Y \right] \right) \right].$$
(28)

Combining the definition of matrix Φ -entropies with (28) immediately gives the following law of total variance:

$$H_{\Phi}(\boldsymbol{Z}) = \mathbb{E}_{Y} \left[H_{\Phi}(\boldsymbol{Z}|Y) \right] + H_{\Phi} \left(\mathbb{E} \left[\boldsymbol{Z}|Y \right] \right).$$
⁽²⁹⁾

Fix $\Phi(u) = u \log u$ and assume that the distribution $\mu \in \mathcal{P}(\mathcal{X})$ is defined on a discrete space \mathcal{X} . If we consider a random matrix ρ_X to be an ensemble of classical-quantum (c-q) states $(\mu, \nu) \triangleq \{(\mu(x), \rho_x)\}_{x \in \mathcal{X}}$, where each $\rho_x \succeq 0$ and Tr $\rho_x = 1$, then its Φ -entropy is related to the *Holevo quantity* of $\{(\mu(x), \rho_x)\}_{x \in \mathcal{X}}$.

$$d \cdot H_{u \log u}(\boldsymbol{\rho}_X) \equiv \sum_{x \in \mathcal{X}} \mu(x) \operatorname{Tr} \left[\boldsymbol{\rho}_x \log \boldsymbol{\rho}_x\right] - \operatorname{Tr} \left[\bar{\boldsymbol{\rho}} \log \bar{\boldsymbol{\rho}}\right] = \sum_{x \in \mathcal{X}} \mu(x) \cdot S\left(\boldsymbol{\rho}_x \| \bar{\boldsymbol{\rho}}\right) =: \chi(\mu, \boldsymbol{\nu}),$$

where $\bar{\boldsymbol{\rho}} = \mathbb{E}_{\mu}[\boldsymbol{\rho}_X] = \sum_{x \in \mathcal{X}} \mu(x) \boldsymbol{\rho}_x$ and $S(\boldsymbol{\rho} \| \boldsymbol{\sigma}) \triangleq \operatorname{Tr} \boldsymbol{\rho}(\log \boldsymbol{\rho} - \log \boldsymbol{\sigma})$ is the quantum relative entropy.

Denote by $\rho_Y \equiv \{\mu'(y), \rho'_y\}_{y \in \mathcal{Y}}$ the resulting random matrix of ρ_X that undergoes a Markov evolution K by the rule:

$$\{\mu(x)\}_{x\in\mathcal{X}} \mapsto \{\mu K(y)\}_{y\in\mathcal{Y}} = \left\{\sum_{x\in\mathcal{X}} \mu(x)K(y|x)\right\}_{y\in\mathcal{Y}} =: \{\mu'(y)\}_{y\in\mathcal{Y}};$$

$$\{\rho_x\}_{x\in\mathcal{X}} \mapsto \{K^*\boldsymbol{\nu}(y)\}_{y\in\mathcal{Y}} = \left\{\sum_{x\in\mathcal{X}} K^*(x|y)\rho_x\right\}_{y\in\mathcal{Y}} =: \{\rho'_y\}_{y\in\mathcal{Y}}.$$
(30)

Note that each ρ'_y can be interpreted as the conditional expectation $\mathbb{E}_{K^*}[\rho_X|Y=y]$, which is a postselection state with the probability law $\{K^*(x|y)\}_{x\in\mathcal{X}}$. We also have the following relationship between the Φ -entropy of ρ_Y and the Holevo quantity of $(\mu', \nu') \triangleq \{(\mu'(y), \rho'_y)\}_{y\in\mathcal{Y}}$:

$$d \cdot H_{u \log u}(\boldsymbol{\rho}_Y) = \sum_{y \in \mathcal{Y}} \mu'(y) \operatorname{Tr} \left[\boldsymbol{\rho}'_y \log \boldsymbol{\rho}'_y \right] - \operatorname{Tr} \left[\overline{\boldsymbol{\rho}'} \log \overline{\boldsymbol{\rho}'} \right] =: \chi(\mu', \boldsymbol{\nu}'), \tag{31}$$

where $\overline{\rho'} = \mathbb{E}_{\mu'}[\rho_Y] = \sum_{y \in \mathcal{Y}} \mu'(y) \rho'_y$.

Now for any $\mu \in \mathcal{P}(\mathcal{X})$ and $K \in \mathcal{M}(Y|X)$, we define the constant:

$$\eta_{\Phi}(\mu, K) \triangleq \sup_{\boldsymbol{\nu}: \chi(\mu, \boldsymbol{\nu}) \neq 0} \frac{\chi(\mu', \boldsymbol{\nu}')}{\chi(\mu, \boldsymbol{\nu})}.$$
(32)

By Jensen's inequality, it can be shown that $0 \le \eta_{\Phi}(\mu, K) \le 1$ (see Lemma 16). Therefore, we relate $\eta_{\Phi}(\mu, K)$ to the following functional inequality of the matrix Φ -entropies.

Proposition 10 (Functional Form for C-Q Ensembles). Fix an admissible pair (μ, K) and let (X, Y) be a random pair with probability law $\mu \otimes K$. Then $\eta_{\Phi}(\mu, K) \leq c$ if and only if the inequality

$$H_{\Phi}[\boldsymbol{f}(X)] \leq \frac{1}{1-c} \mathbb{E} \left(H_{\Phi}[\boldsymbol{f}(X)|Y] \right)$$
(33)

holds for all non-constant classical-quantum states $f : \mathcal{X} \to \mathcal{Q}(\mathbb{C}^d)$, where we denote by $\mathcal{Q}(\mathbb{C}^d)$ the set of density operators on \mathbb{C}^d . In particular, Eq. (33) can be expressed in terms of Holevo quantities:

$$\chi(\mu, \boldsymbol{\nu}) \le \frac{1}{1-c} \mathbb{E}_Y \left[\chi(K^*, \boldsymbol{\nu} | Y) \right]$$
(34)

where the expectation \mathbb{E}_Y is taken with respect to $\{\mu K(y)\}_{y \in \mathcal{Y}}$.

Moreover,

$$\eta_{\Phi}(\mu, K) = 1 - \inf\left\{\frac{\mathbb{E}\left[H_{\Phi}(\boldsymbol{f}(X)|Y)\right]}{H_{\Phi}(\boldsymbol{f}(X))} : \boldsymbol{f} \neq \text{const}\right\}.$$
(35)

Proof. The inequality $\chi(\mu', \nu') \leq c \cdot \chi(\mu, \nu)$ is equivalent to

$$H_{\Phi}(K^*\boldsymbol{f}(Y)) \leq cH_{\Phi}(\boldsymbol{f}(X))$$

= $c\left(\mathbb{E}\left[H_{\Phi}(\boldsymbol{f}(X)|Y)\right] + H_{\Phi}\left(\mathbb{E}\left[\boldsymbol{f}(X)|Y\right]\right)\right)$
= $c\left(\mathbb{E}\left[H_{\Phi}(\boldsymbol{f}(X)|Y)\right] + H_{\Phi}\left(K^*\boldsymbol{f}(Y)\right)\right),$ (36)

where we use the identity of the law of total variance, Eq. (29), and the property of the backward channel, Eq. (27), from which we obtain

$$H_{\Phi}(K^*\boldsymbol{f}(Y)) \le \frac{c}{1-c} \mathbb{E}\left[H_{\Phi}(\boldsymbol{f}(X)|Y)\right],\tag{37}$$

and hence,

$$H_{\Phi}[\boldsymbol{f}(X)] = \mathbb{E}\left[H_{\Phi}(\boldsymbol{f}(X)|Y)\right] + H_{\Phi}\left(K^{*}\boldsymbol{f}(Y)\right) \leq \frac{1}{1-c}\mathbb{E}\left(H_{\Phi}[\boldsymbol{f}(X)|Y]\right).$$
(38)

Raginsky showed, in recent work [53, 17], that if $f = d\nu/d\mu$ (i.e. a Radon-Nikodym derivative), then $K^*f = \frac{d(\nu K)}{d(\mu K)}$. Moreover, the constant $\eta_{\Phi}(\mu, K)$ in Eq. (32) corresponds to the (classical) strong data processing inequality (SDPI):

$$\eta_{\Phi}(\mu, K) \triangleq \sup_{\nu \neq \mu} \frac{D(\nu K, \mu K)}{D(\nu, \mu)},\tag{39}$$

where $D(\nu, \mu)$ is the classical Kullback-Leibler divergence of μ and ν . We remark that Proposition 10 can be viewed as a generalization of Raginshky's SDPI result to case of quantum ensembles undergoing the Markov evolution K described in Eq. (30).

5. Conclusions

In this paper, we extend the work of Gross [14] to study the Φ -Sobolev and Poincaré inequalities on matrix-valued functions. The uncertainty measure adopted in this work is the matrix Φ -entropy [62], which interpolates between the variance and conventional entropies of random matrices. The Dirichlet energy is defined as the average of local influences on every bit position. We note, that if the considered domain is a Boolean hypercube (i.e. $\mathcal{X} = \{0, 1\}^n$), then the our notion coincides with the Dirichlet form induced by the Markov jumping process [42]. Our results generalise the classical functional inequalities to the matrix Poincaré inequality for separable convex functions and Gaussian unitary ensembles. Moreover, we establish the matrix Φ -Sobolev inequalities for symmetric Bernoulli and standard Gaussian distributions. Unlike its classical counterpart [68], the derived inequality is defective, which shows the matrix version is more involved, but it reduces to the classical case when d = 1.

The random matrix framework has immediate applications in quantum information theory and mathematics. For example, by relating the matrix Φ -entropy to the celebrated Holevo quantity, we obtain a formula for the strong data processing inequality. In a follow-up work [42], we are able to upper bound the convergence rate of the dynamical evolutions of a quantum ensemble by employing the matrix Efron-Stein inequality and a modified log-Sobolev inequality. Furthermore, the studied model naturally occurs in the probabilistic context of matrix-valued stochastic processes [43, 69]. Solving the matrix functional inequalities of the Markovian matrix-valued processes provides a way to characterize their long-term behaviours.

APPENDIX A. MISCELLANEOUS LEMMAS

Lemma 11. Let X be a random matrix taking values in \mathbb{M}^{sa} , and let Y be independently and identically distributed as X. Then for each natural number $q \geq 1$,

$$\mathbb{E}\left[|\boldsymbol{X} - \mathbb{E}\boldsymbol{X}|^{q}\right] = \mathbb{E}\left[(\boldsymbol{X} - \mathbb{E}\boldsymbol{X})_{+}^{q}\right] + \mathbb{E}\left[(\boldsymbol{X} - \mathbb{E}\boldsymbol{X})_{-}^{q}\right]$$
(40)

and

$$\frac{1}{2}\mathbb{E}\left[|\boldsymbol{X}-\boldsymbol{Y}|^{q}\right] = \mathbb{E}\left[(\boldsymbol{X}-\boldsymbol{Y})_{+}^{q}\right] = \mathbb{E}\left[(\boldsymbol{X}-\boldsymbol{Y})_{-}^{q}\right]$$
(41)

In particular,

$$\mathbb{E}\left[\left(\boldsymbol{X} - \mathbb{E}\boldsymbol{X}\right)^{2}\right] = \frac{1}{2}\mathbb{E}\left[\left(\boldsymbol{X} - \boldsymbol{Y}\right)^{2}\right].$$
(42)

Proof. For each realisation X of \mathbf{X} in \mathbb{M}^{sa} , $X = X_+ - X_-$ for some $X_+, X_- \succeq 0$ and $X_+X_- = \mathbf{0}$. Slightly abusing the notation, we hence use \mathbf{X}_+ and \mathbf{X}_- to denote the positive and negative decomposition of their realisations of \mathbf{X} .

Therefore, for each natural number $q \ge 1$,

$$\mathbb{E}\left[|\boldsymbol{X} - \mathbb{E}\boldsymbol{X}|^{q}\right] = \mathbb{E}\left[\left((\boldsymbol{X} - \mathbb{E}\boldsymbol{X})_{+} + (\boldsymbol{X} - \mathbb{E}\boldsymbol{X})_{-}\right)^{q}\right] = \mathbb{E}\left[(\boldsymbol{X} - \mathbb{E}\boldsymbol{X})_{+}^{q}\right] + \mathbb{E}\left[(\boldsymbol{X} - \mathbb{E}\boldsymbol{X})_{-}^{q}\right].$$

Likewise, we have

$$\frac{1}{2}\mathbb{E}\left[|\boldsymbol{X}-\boldsymbol{Y}|^{q}\right] = \frac{1}{2}\mathbb{E}\left[\left((\boldsymbol{X}-\boldsymbol{Y})_{+}+(\boldsymbol{Y}-\boldsymbol{X})_{+}\right)^{q}\right] = \mathbb{E}\left[\left(\boldsymbol{X}-\boldsymbol{Y}\right)_{+}^{q}\right].$$

The last line follows since Y is an identical copy of X.

Following the same reasoning, we have $|\mathbf{X}| = \mathbf{X}_{-} + (-\mathbf{X})_{-}$, and thus $\frac{1}{2}\mathbb{E}[|\mathbf{X} - \mathbf{Y}|^q] = \mathbb{E}[(\mathbf{X} - \mathbf{Y})^q_{-}]$. Finally, Eq. (42) follows from elementary calculations:

$$\frac{1}{2}\mathbb{E}\left[\left(\boldsymbol{X}-\boldsymbol{Y}\right)^{2}\right] = \frac{1}{2}\mathbb{E}\left[\boldsymbol{X}^{2}-\boldsymbol{X}\boldsymbol{Y}-\boldsymbol{Y}\boldsymbol{X}+\boldsymbol{Y}^{2}\right] = \mathbb{E}\left[\left(\boldsymbol{X}-\mathbb{E}\boldsymbol{X}\right)^{2}\right].$$

Lemma 12 (Central Limit Theorem of Gaussian Unitary Ensembles). Let $\{\epsilon_j\}_j$ be a series of Rademacher variables, and let $\{W_j\}_j$, $\{W'_j\}_j$ be $d \times d$ matrices whose entries are sampled independently from the

Rademacher variables. Let

$$m{Y}_j = rac{\left(m{W}_j + \mathrm{i} \cdot m{W}'_j
ight) + \left(m{W}_j + \mathrm{i} \cdot m{W}'_j
ight)^{\intercal}}{2},$$

and $\mathbf{S}_m \triangleq \frac{1}{\sqrt{m}} \sum_{j=1}^m \epsilon_j \mathbf{Y}_j$, where $\{\epsilon_j\}_j$ are Rademacher variables again. If m tends to infinity, then \mathbf{S}_m converges in distribution to a $d \times d$ matrix in the Gaussian unitary ensemble.

Proof. It is clear from the central limit theorem that the diagonal entries converge to a standard real Gaussian variable, while the upper-triangular entries converge to a complex Gaussian variables with zero mean and unit variance. Next, we show that the correlation between any (non-identical) entry vanishes as m goes to infinity. That is, for every $(k, l) \neq (k', l')$

$$\mathbb{E}_{\epsilon_1,...,\epsilon_m} \left[S_m^{(kl)} S_m^{(k'l')} \right] = \frac{1}{m} \sum_{j=1}^m Y_j^{(kl)} Y_j^{(k'l')},$$

from which we apply the strong law of large numbers to obtain

$$\lim_{m \to \infty} \frac{1}{m} \sum_{j=1}^{m} Y_j^{(kl)} Y_j^{(k'l')} = \mathbb{E}\left[Y \cdot Y'\right] = \mathbb{E}\left[Y\right] \cdot \mathbb{E}\left[Y'\right] = 0 \quad \text{almost surely,}$$

where we denote by Y (resp. Y') the random variable that the sequences $\{Y_j^{(kl)}\}_j$ (resp. $\{Y_j^{(k'l')}\}_j$) are sampled from. It is easy to see that Y and Y' are independent zero-mean random variables. Therefore, the entries are mutually independent and $\lim_{m\to\infty} S_m$ belongs to the Gaussian unitary ensemble.

Lemma 13 (Parseval's Identity for Matrix-Valued Functions). For every matrix-valued function $f : \{0,1\}^n \to \mathbb{M}_d$, we have the following identity

$$\mathbb{E}\left[\boldsymbol{f}(X)^2\right] = \sum_{S \subseteq [n]} \widehat{\boldsymbol{f}}(S)^2,$$

where the expectation is taken uniformly over all $X \in \{0,1\}^n$.

Proof. With the Fourier expansion of the matrix-valued function f, it follows that

$$\mathbb{E}\left[\boldsymbol{f}(X)^{2}\right] = \mathbb{E}\left[\boldsymbol{f}(X) \cdot \left(\sum_{S \subseteq [n]} \widehat{\boldsymbol{f}}(S) \chi_{S}(X)\right)\right] = \sum_{S \subseteq [n]} \widehat{\boldsymbol{f}}(S) \cdot \mathbb{E}\left[\boldsymbol{f}(X) \chi_{S}(X)\right] = \sum_{S \subseteq [n]} \widehat{\boldsymbol{f}}(S)^{2}.$$

Lemma 14. With the prevailing assumptions, and every $f: \{0,1\}^n \to \mathbb{M}_d^{sa}$, we have

$$\sum_{S\subseteq[n]} \overline{\mathrm{tr}}\left[|S|\widehat{f}(S)^2\right] = \mathcal{E}(f).$$

Proof. For every *n*-tuple $x \triangleq (x_1, \ldots, x_n) \in \{0, 1\}^n$, denote $\overline{x}^{(i)} \triangleq (x_1, \ldots, x_{i-1}, 1 - x_i, x_{i+1}, \ldots, x_n)$. For every $i \in [n]$, introduce the matrix-valued function $g_i(x) = \frac{f(x) - f(\overline{x}^{(i)})}{2}$. Then, for every $S \subseteq [n]$, it can be observed that

$$\widehat{\boldsymbol{g}}_{i}(S) = \mathbb{E}\left[\boldsymbol{g}_{i}(X)\chi_{S}(X)\right] = \frac{1}{2}\mathbb{E}\left[\left(\boldsymbol{f}(X) - \boldsymbol{f}(\overline{X}^{(i)})\right) \cdot (-1)^{\sum_{j \in S} X_{j}}\right] = \begin{cases} 0 & \text{if } i \notin S \\ \widehat{\boldsymbol{f}}(S) & \text{if } i \in S \end{cases}$$

Apply Parseval's identity, Lemma 13 to obtain

$$\mathbb{E}\left[\boldsymbol{g}_{i}(X)^{2}\right] = \sum_{S \subseteq [n]} \widehat{\boldsymbol{g}}_{i}(S)^{2} = \sum_{S: i \in S} \widehat{\boldsymbol{f}}(S)^{2}.$$

Finally, since X is uniformly distributed, $\mathcal{E}(f)$ can be rewritten as

$$\mathcal{E}(\boldsymbol{f}) = \frac{1}{2} \overline{\operatorname{tr}} \mathbb{E} \left[\sum_{i=1}^{n} \left(\boldsymbol{f}(X) - \boldsymbol{f}\left(\widetilde{X}^{(i)}\right) \right)^{2} \right] = \frac{1}{4} \overline{\operatorname{tr}} \mathbb{E} \left[\sum_{i=1}^{n} \left(\boldsymbol{f}(X) - \boldsymbol{f}\left(\overline{X}^{(i)}\right) \right)^{2} \right]$$
$$= \sum_{i=1}^{n} \overline{\operatorname{tr}} \mathbb{E} \left[\boldsymbol{g}_{i}(X)^{2} \right] = \sum_{i=1}^{n} \sum_{S:i\in S} \overline{\operatorname{tr}} \left[\widehat{\boldsymbol{f}}(S)^{2} \right] = \sum_{S\subseteq [n]} \overline{\operatorname{tr}} \left[|S| \widehat{\boldsymbol{f}}(S)^{2} \right].$$

This completes the proof.

Lemma 15. Let \mathbf{Z} be a random matrix taking values in \mathbb{M}^+ such that $\|\mathbf{Z}\|_{\infty} < \infty$. For $p \in [1,2)$, we define the matrix-valued *p*-variance of \mathbf{Z} by $\operatorname{Var}_p[\mathbf{Z}] \triangleq \mathbb{E}[\mathbf{Z}^2] - (\mathbb{E}[\mathbf{Z}^p])^{2/p}$. It follows that

$$\lim_{p \to 2^{-}} \frac{\operatorname{Var}_{p}[\boldsymbol{Z}]}{2-p} = \frac{1}{2} \mathbb{E} \Big[\boldsymbol{Z}^{2} \log \boldsymbol{Z}^{2} \Big] - \frac{1}{2} \mathbb{E} \big[\boldsymbol{Z}^{2} \big] \cdot \log \mathbb{E} \big[\boldsymbol{Z}^{2} \big].$$

Proof. We first prove a formula for the matrix differentiation. Denote by $\mathbf{A} = \mathbf{A}(p)$ a Hermitian matrix which depends on the real parameter p. Then we aim to solve the derivative of $\mathbf{A}^{2/p}$ with respect to p. Let $\mathbf{Y} = \mathbf{A}^{2/p}$. Then $\log \mathbf{Y} = \log \mathbf{A} \cdot 2/p$. Differentiating on both sides with respect to p and applying the chain rule of the Fréchet derivatives, the above expression leads to

$$\frac{\mathrm{d}}{\mathrm{d}p}\log \mathbf{Y} = \int_0^\infty (s\mathbf{I} + \mathbf{Y})^{-1} \cdot \frac{\mathrm{d}}{\mathrm{d}p} \mathbf{Y} \cdot (s\mathbf{I} + \mathbf{Y})^{-1} \mathrm{d}s = \frac{\mathrm{d}}{\mathrm{d}p}\log \mathbf{A} \cdot 2/p$$

$$= -\frac{2}{p^2}\log \mathbf{A} + \frac{2}{p} \int_0^\infty (t\mathbf{I} + \mathbf{A})^{-1} \cdot \frac{\mathrm{d}}{\mathrm{d}p} \mathbf{A} \cdot (t\mathbf{I} + \mathbf{A})^{-1} \mathrm{d}t.$$
(43)

Note that $\mathsf{T}_{\boldsymbol{D}}(\boldsymbol{K}) \triangleq \int_0^\infty (s\boldsymbol{I} + \boldsymbol{D})^{-1} \boldsymbol{K} (s\boldsymbol{I} + \boldsymbol{D})^{-1} \mathrm{d}s$ is called the *Bogoliubov-Kubo-Mori operator* and its inverse is well-known to be $\mathsf{T}_{\boldsymbol{D}}^{-1}(\boldsymbol{L}) = \int_0^1 \boldsymbol{D}^s \boldsymbol{L} \boldsymbol{D}^{1-s} \mathrm{d}s$ (see e.g. [70, Appendix C.2]), from which Eq. (43) yields

$$\frac{\mathrm{d}}{\mathrm{d}p} \mathbf{Y} = \int_0^1 \mathbf{Y}^s \left[-\frac{2}{p^2} \log \mathbf{A} + \frac{2}{p} \int_0^\infty (t\mathbf{I} + \mathbf{A})^{-1} \cdot \frac{\mathrm{d}}{\mathrm{d}p} \mathbf{A} \cdot (t\mathbf{I} + \mathbf{A})^{-1} \mathrm{d}t \right] \mathbf{Y}^{1-s} \,\mathrm{d}s$$
$$= -\frac{2}{p^2} \mathbf{A}^{2/p} \cdot \log \mathbf{A} + \frac{2}{p} \int_0^1 \int_0^\infty \mathbf{A}^{2s/p} (t\mathbf{I} + \mathbf{A})^{-1} \cdot \frac{\mathrm{d}}{\mathrm{d}p} \mathbf{A} \cdot (t\mathbf{I} + \mathbf{A})^{-1} \mathbf{A}^{2/p-2s/p} \,\mathrm{d}t \,\mathrm{d}s.$$

Now, by taking $\mathbf{A} \equiv \mathbb{E}[\mathbf{Z}^p]$ we have $\frac{\mathrm{d}}{\mathrm{d}p}\mathbf{A} = \frac{\mathrm{d}}{\mathrm{d}p}\mathbb{E}[\mathbf{Z}^p] = \mathbb{E}[\mathbf{Z}^p \cdot \log \mathbf{Z}]$ and

$$\frac{\mathrm{d}}{\mathrm{d}p} \left(\mathbb{E} \left[\boldsymbol{Z}^{p} \right] \right)^{2/p} = -\frac{2}{p^{2}} \left(\mathbb{E} \left[\boldsymbol{Z}^{p} \right] \right)^{2/p} \log \mathbb{E} \left[\boldsymbol{Z}^{p} \right]
+ \frac{2}{p} \int_{0}^{1} \int_{0}^{\infty} \boldsymbol{A}^{2s/p} (t\boldsymbol{I} + \boldsymbol{A})^{-1} \cdot \mathbb{E} \left[\boldsymbol{Z}^{p} \cdot \log \boldsymbol{Z} \right] \cdot (t\boldsymbol{I} + \boldsymbol{A})^{-1} \boldsymbol{A}^{2/p-2s/p} \, \mathrm{d}t \, \mathrm{d}s.$$
(44)

Finally, we are ready to prove our claim. L'Hôpital's rule implies

$$\begin{split} \lim_{p \to 2^{-}} \frac{\mathbf{Var}_{p}[\mathbf{Z}]}{2-p} &= \frac{\mathrm{d}}{\mathrm{d}p} \Big(\mathbb{E}[\mathbf{Z}^{p}] \Big)^{2/p} \Big|_{p=2} \\ &= -\frac{1}{2} \mathbb{E}[\mathbf{Z}^{2}] \cdot \log \mathbb{E}[\mathbf{Z}^{2}] + \int_{0}^{1} \int_{0}^{\infty} \mathbf{A}^{s} (t\mathbf{I} + \mathbf{A})^{-1} \cdot \mathbb{E}[\mathbf{Z}^{p} \cdot \log \mathbf{Z}] \cdot (t\mathbf{I} + \mathbf{A})^{-1} \mathbf{A}^{1-s} \, \mathrm{d}t \, \mathrm{d}s \\ &= \frac{1}{2} \mathbb{E}[\mathbf{Z}^{2} \log \mathbf{Z}^{2}] - \frac{1}{2} \mathbb{E}[\mathbf{Z}^{2}] \cdot \log \mathbb{E}[\mathbf{Z}^{2}], \end{split}$$

completing the proof.

Lemma 16. Fix sample spaces \mathcal{X} and \mathcal{Y} . For every distribution $\mu \in \mathcal{P}(\mathcal{X})$, Markov kernel $K \in \mathcal{M}(\mathcal{Y}|\mathcal{X})$ and matrix-valued function $f : \mathcal{X} \to \mathbb{M}_d^+$, we have the following inequality:

$$H_{\Phi}(K^{*}\boldsymbol{f}) = \overline{\operatorname{tr}}\left[\mathbb{E}_{\mu K}\left[\Phi(K^{*}\boldsymbol{f})\right] - \Phi\left(\mathbb{E}_{\mu K}\left[K^{*}\boldsymbol{f}\right]\right)\right] \leq \overline{\operatorname{tr}}\left[\mathbb{E}_{\mu}\Phi(\boldsymbol{f}) - \Phi\left(\mathbb{E}_{\mu}\boldsymbol{f}\right)\right] = H_{\Phi}(\boldsymbol{f}),$$

K and *K*^{*} are defined in Eq. (24) and (26)

where μK and K^* are defined in Eqs. (24) and (26).

Proof. We first observe that Jensen's inequality [71, Section 5] holds for all convex functions Φ : $\overline{\operatorname{tr}} [K^* \Phi(f)] \geq \overline{\operatorname{tr}} [\Phi(K^* f)]$. After taking expectation with respect to μK , direct calculation shows that

$$\overline{\operatorname{tr}} \mathbb{E}_{\mu K} \left[K^* \Phi \left(\boldsymbol{f} \right) \right] = \sum_{y \in \mathcal{Y}} \mu K(y) \cdot \overline{\operatorname{tr}} \left[K^* \Phi \circ \boldsymbol{f}(y) \right] = \sum_{y \in \mathcal{Y}} \mu K(y) \cdot \overline{\operatorname{tr}} \left[\sum_{x \in \mathcal{X}} \frac{K(y|x)\mu(x)}{\mu K(y)} \Phi \left(\boldsymbol{f}(x) \right) \right]$$
$$= \sum_{x \in \mathcal{X}} \mu(x) \overline{\operatorname{tr}} \left[\Phi \left(\boldsymbol{f}(x) \right) \right] = \overline{\operatorname{tr}} \mathbb{E}_{\mu} \left[\Phi(f) \right] \ge \sum_{y \in \mathcal{Y}} \mu K(y) \cdot \overline{\operatorname{tr}} \left[\Phi \left(K^* \boldsymbol{f} \right) \right]$$
$$= \overline{\operatorname{tr}} \mathbb{E}_{\mu K} \left[\Phi(K^* \boldsymbol{f}) \right]$$

(note that we freely interchange the order of trace and expectation by Fubini's theorem). Together with the fact that $\mathbb{E}_{\mu K}[K^* f] = \mathbb{E}_{\mu} f$, we complete our claim.

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