

Asymptotic mutual information in quadratic estimation problems over compact groups

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Abstract

Motivated by applications to group synchronization and quadratic assignment on random data, we study a general problem of Bayesian inference of an unknown “signal” belonging to a high-dimensional compact group, given noisy pairwise observations of a featurization of this signal. We establish a quantitative comparison between the signal-observation mutual information in any such problem with that in a simpler model with linear observations, using interpolation methods. For group synchronization, our result proves a replica formula for the asymptotic mutual information and Bayes-optimal mean-squared-error. Via analyses of this replica formula, we show that the conjectural phase transition threshold for computationally-efficient weak recovery of the signal is determined by a classification of the real-irreducible components of the observed group representation(s), and we fully characterize the information-theoretic limits of estimation in the example of angular/phase synchronization over $\mathbb{S}\mathbb{O}(2)/\mathbb{U}(1)$. For quadratic assignment, we study observations given by a kernel matrix of pairwise similarities and a randomly permuted and noisy counterpart, and we show in a bounded signal-to-noise regime that the asymptotic mutual information coincides with that in a Bayesian spiked model with i.i.d. signal prior.

1 Introduction

The estimation of a low-rank matrix in a noisy channel is a fundamental problem in statistical inference, which has received much attention in recent years [DAM16, KXZ16, DMK⁺16, EAK18, LM19, BM19, BR20]. In this work, we are motivated by two applications that may be viewed as extensions or variants of this problem:

- In *group synchronization*, we wish to estimate a collection of elements $\mathbf{g}_{*1}, \dots, \mathbf{g}_{*N} \in \mathcal{G}$ from a known compact group \mathcal{G} , given noisy observations of their pairwise alignments

$$\mathbf{y}_{ij} = \mathbf{g}_{*i} \mathbf{g}_{*j}^{-1} + \text{Gaussian noise.}$$

Examples include synchronization problems over the binary group $\mathbb{Z}/2\mathbb{Z}$ with application to community detection in networks [DAM16], over $\mathbb{S}\mathbb{O}(2)$ (or equivalently $\mathbb{U}(1)$ in the complex domain) with application to angular and phase synchronization [Sin11], over $\mathbb{S}\mathbb{O}(3)$ with application to image registration and cryo-electron microscopy [BCLS20], and over the symmetric group \mathbb{S}_k with application to multi-way matching [PKS13].

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- In *quadratic assignment*, we wish to estimate a permutation $\pi \in \mathbb{S}_N$ (the symmetric group on N elements) that minimizes a cost function

$$\sum_{1 \leq i < j \leq N} (y_{ij} - a_{\pi(i)\pi(j)})^2$$

for two sets of pairwise similarities $\{a_{ij}\}_{1 \leq i < j \leq N}$ and $\{y_{ij}\}_{1 \leq i < j \leq N}$ between N objects. We study a statistical setting where $a_{ij} = \kappa(x_i, x_j)$ is the evaluation of a symmetric kernel function $\kappa(\cdot, \cdot)$ on samples x_1, \dots, x_N , and the above quadratic cost arises as the log-likelihood in a model

$$y_{ij} = a_{\pi_*(i)\pi_*(j)} + \text{Gaussian noise}$$

for an unknown true permutation $\pi_* \in \mathbb{S}_N$. This is a Gaussian-noise analogue of some recently studied models of graph matching on random geometric graphs [WWXY22, GL24, LA24], here with independent noise for each measurement pair (i, j) rather than for each underlying sample x_1, \dots, x_N .

These two seemingly different problems share a common underlying structure of inferring an unknown element $G_* \in \mathcal{G}_N$ of a high-dimensional group from noisy pairwise observations, where $\mathcal{G}_N \equiv \mathcal{G}^N$ is an N -fold product group in synchronization, and $\mathcal{G}_N \equiv \mathbb{S}_N$ is the symmetric group in quadratic assignment. Other applications having this structure include problems of ranking from pairwise comparisons [FH10, NOS12], and Procrustes hyperalignment problems that arise in analyses of functional MRI data [HGC⁺11, LR12].

In this work, we introduce and study a general formulation for such problems in a Bayesian setting, where pairwise measurements

$$\mathbf{y}_{ij} = \phi(G_*)_i \bullet \phi(G_*)_j + \text{Gaussian noise for } 1 \leq i < j \leq N \tag{1}$$

are observed corresponding to a featurization $\phi(\cdot)$ of G_* belonging to a compact group \mathcal{G}_N , assumed to have Haar-uniform prior distribution. The Hamiltonian of the Bayes posterior law is a \mathcal{G}_N -indexed Gaussian process whose mean and covariance are determined by a corresponding overlap function

$$Q(G, G') = N^{-1} \sum_{i=1}^N \phi(G)_i \otimes \phi(G')_i.$$

We refer to Section 2 for details of this setup. In the context of this general model as well as the aforementioned synchronization and quadratic assignment applications of interest, our work makes the following contributions:

1. We analyze the mutual information between the latent group element $G_* \in \mathcal{G}_N$ and the observations $\{\mathbf{y}_{ij}\}_{i < j}$ in general models of the form (1), showing that this admits an approximation in terms of the mutual information in a linear observation model

$$\mathbf{y}_i = \mathbf{q}^{1/2} \phi(G_*)_i + \text{Gaussian noise for } i = 1, \dots, N$$

defined by a suitable element \mathbf{q} of the overlap space. The approximation error is small when the overlap space has small covering number, encompassing scenarios where the signal component of the pairwise measurements has low effective rank.

Our proof of this result uses interpolation arguments that have been successfully developed and applied to establish replica formulas in problems of low-rank matrix estimation [KXZ16, EAK18, BM19]. In

particular, we apply an elegant method of [EAK18] for proving an upper bound on the free energy (i.e. lower bound on the mutual information) by interpolating on the Franz-Parisi potential at each fixed overlap, adapting this method to settings where the prior law of $G_* \in \mathcal{G}_N$ has group symmetry but may not necessarily decompose as a product of i.i.d. components.

2. Specialized to group synchronization, we provide a rigorous proof of a replica formula for the asymptotic signal-observation mutual information and Bayes-optimal minimum mean-squared error (MMSE) in a bounded SNR regime. A version of this replica formula in a model with complex observations was stated in [PWBM18], which also proposed Approximate Message Passing algorithms for inference.

We obtain a complete characterization of the optimization landscape of the replica potential for (single-channel) $\mathbb{SO}(2)/\mathbb{U}(1)$ -synchronization, implying a characterization of the information-theoretic limits of inference. More generally, for any group, we analyze the stability of the overlap $\mathbf{q} = \mathbf{0}$ as a critical point of the replica potential, which conjecturally corresponds to the feasibility of non-trivial signal estimation (i.e. weak recovery) by polynomial-time algorithms [LKZ17, LM19]. We show that the phase transition threshold for local optimality of $\mathbf{q} = \mathbf{0}$ is determined by the SNR parameters of an equivalent multi-channel model with real-irreducible group representations, together with a classification of these representations based on their further reduction into complex-irreducible components.

3. Specialized to quadratic assignment where $a_{ij} = \kappa(x_i, x_j)$ and $y_{ij} = a_{\pi_*(i)\pi_*(j)} + \text{Gaussian noise}$, our result implies that the mutual information is related to that in a linear observation model

$$\mathbf{y}_i = \mathbf{q}^{1/2} \phi(x_{\pi_*(i)}) + \text{Gaussian noise}$$

where $\phi(\cdot)$ is a feature map defined by eigenfunctions of the kernel $\kappa(\cdot, \cdot)$. This linear model, although not independent across components $i = 1, \dots, N$, is well-studied as an oracle model in the literature on compound decision problems and empirical Bayes estimation [HR55, GR09, JZ09, PW21]. We deduce from results of this literature that in a bounded SNR regime, if the empirical distribution of $\{x_i\}_{i=1}^N$ converges to a limit law ρ , then the asymptotic mutual information between π_* and $\{a_{ij}, y_{ij}\}_{i < j}$ coincides with the mutual information in a low-rank matrix estimation model having i.i.d. prior ρ for its signal components.

We present the detailed setting and results of the general model in Section 2, the specialization to group synchronization in Section 3, and the specialization to random quadratic assignment in Section 4.

1.1 Further related literature

Interpolation methods and overlap concentration. Gaussian interpolation techniques for computing free energies in spin glass models were brought to prominence by Guerra [Gue03], and have since been extended and applied to characterize the fundamental limits of inference in many Bayesian statistical problems with planted signals, including [KM09, KXZ16, DMK⁺16, EAK18, LM19, BM19, BKM⁺19]. In Bayesian inference problems, obtaining a tight upper bound for the log-partition-function (i.e. free energy) is oftentimes more intricate than the lower bound; this was achieved in low-rank matrix estimation problems using an Aizenman-Sims-Starr scheme in [LM19] and an adaptive interpolation method in [BM19]. Our proofs build upon a different method in [EAK18] of analyzing the large deviations of the overlap between a posterior sample and the planted signal, by bounding the Franz-Parisi potential [FP97], i.e. the free energy restricted to configurations having overlap values in a narrow range. For the high-temperature region of the classical

Sherrington-Kirkpatrick model, this is also related to the analysis carried out in [Tal11, Theorem 13.4.2]. Large deviations of the overlap have also been studied recently for low-rank matrix estimation models outside the replica-symmetric setting, under a mismatched prior and noise distribution, in [GKKZ23].

Group synchronization. Angular synchronization problems over $\mathbb{S}\mathbb{O}(2)$ were introduced in [Sin11], and subsequently formulated and studied in settings of general groups in [Ban15, BCLS20]. The specific examples of $\mathbb{Z}/2\mathbb{Z}$ -synchronization [DAM16, BBV16, MS16, JMRT16, FMM21, LW22, CFM23, LFW23], angular/phase synchronization [Bou16, BBS17, LYMCS17, ZB18, GZ19, GZ22], and synchronization problems over the orthogonal and symmetric groups [CLS12, PKS13, GZ21, Lin22b, Lin22a, Zha22, GZ23, Lin23, NZ23] have each received substantial attention in their own right. Much of this literature focuses on the performance of spectral, semidefinite-programming (SDP), and/or nonconvex optimization methods for estimation, and their associated guarantees for exact recovery or optimal estimation rates in regimes of growing SNR.

Closer to our work are the (mostly non-rigorous) results of [JMRT16, PWBM18] which study synchronization problems in bounded SNR regimes, the former analyzing Bayesian, maximum-likelihood, and SDP approaches to inference via the cavity method in the $\mathbb{Z}/2\mathbb{Z}$ - and $\mathbb{U}(1)$ -synchronization models, and the latter introducing an Approximate Message Passing algorithm for Bayes-optimal inference in general synchronization models with multiple observation channels corresponding to distinct complex-irreducible group representations. Our results formalize some of the findings of this latter work [PWBM18] in a similar model having real observations, and are also complementary to analyses of the free energy for general synchronization problems that were carried out in [PWBM16] using a second-moment-method approach.

Quadratic assignment. The quadratic assignment problem was introduced in [KB57], and its behavior on several models of random data has been investigated in [Bur84, FVHRK85, Rhe91]. Statistical applications of quadratic assignment and convex relaxations thereof for estimating latent vertex matchings between random graphs have been studied more recently in [ZBV08, ABK15, LFF⁺15, FMWX23a, FMWX23b], in the context of a broader literature on algorithms and fundamental limits of inference for random graph matching problems [CK17, CKMP20, GM20, DMWX21, Gan22, GMS22, WXY22, HM23, DD23, MRT23, MWXY23]. We study in this work a quadratic assignment problem with random data matrices of low effective rank, bearing similarity to matching problems between random geometric graphs recently considered in [WWXY22, GL24, LA24], and to analyses of related linear matching problems in [CD16, DCK19, KNW22]. Our analyses here pertain to a bounded SNR regime where consistent estimation of the latent permutation/matching is not possible, and where we instead show an exact asymptotic equivalence between the signal-observation mutual information with that in a low-rank matrix estimation model with i.i.d. signal prior.

2 General model and results

Consider a compact group \mathcal{G}_N , a (N -dependent) featurization $\phi : \mathcal{G}_N \rightarrow \mathcal{H}^N$ with “feature” space \mathcal{H} , and a bilinear map $\bullet : \mathcal{H} \times \mathcal{H} \rightarrow \mathcal{K}$ with “observation” space \mathcal{K} , where \mathcal{H}, \mathcal{K} are finite-dimensional real vector spaces endowed with the inner-products $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ and $\langle \cdot, \cdot \rangle_{\mathcal{K}}$. We study a general observation model in which, for an unknown parameter $G_* \in \mathcal{G}_N$ of interest, we observe

$$\mathbf{y}_{ij} = \phi(G_*)_i \bullet \phi(G_*)_j + \sqrt{N} \mathbf{z}_{ij} \text{ for each } 1 \leq i < j \leq N. \quad (2)$$

Here $\{\mathbf{z}_{ij}\}_{i<j}$ are i.i.d. standard Gaussian noise vectors in \mathcal{K} (i.e. having i.i.d. $\mathcal{N}(0,1)$ components in any orthonormal basis of \mathcal{K}).¹

In this work, we will focus on a Bayesian setting where G_* has Haar-uniform prior $G_* \sim \text{Haar}(\mathcal{G}_N)$. Denote the combined observations as $Y = \{\mathbf{y}_{ij}\}_{i<j}$. Bayes-optimal inference for G_* is then based on the posterior density (with respect to Haar measure)

$$p(G | Y) \propto \exp \left(-\frac{1}{2N} \sum_{1 \leq i < j \leq N} \|\mathbf{y}_{ij} - \phi(G)_i \bullet \phi(G)_j\|_{\mathcal{K}}^2 \right) \propto \exp H(G; Y), \quad (3)$$

where we expand the square and define the Hamiltonian

$$H(G; Y) = -\frac{1}{2N} \sum_{1 \leq i < j \leq N} \|\phi(G)_i \bullet \phi(G)_j\|_{\mathcal{K}}^2 + \frac{1}{N} \sum_{1 \leq i < j \leq N} \langle \phi(G)_i \bullet \phi(G)_j, \mathbf{y}_{ij} \rangle_{\mathcal{K}}. \quad (4)$$

We denote its associated free energy

$$\mathcal{F}_N = \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp H(G; Y). \quad (5)$$

Here, \mathbb{E}_G is the expectation over a uniform element $G \sim \text{Haar}(\mathcal{G}_N)$, and $\mathbb{E}_{G_*, Z}$ is over the independent signal $G_* \sim \text{Haar}(\mathcal{G}_N)$ and Gaussian noise vectors $Z = \{\mathbf{z}_{ij}\}_{i<j}$ which define Y .

We assume a model structure in which there exists a complementary bilinear map $\otimes : \mathcal{H} \times \mathcal{H} \rightarrow \mathcal{L}$ to an ‘‘overlap’’ space \mathcal{L} , such that \mathcal{G}_N , ϕ , \bullet , and \otimes satisfy the following properties.

Assumption 2.1. (a) \mathcal{G}_N is a compact group, $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ is a finite-dimensional (real) inner-product space, and $\phi : \mathcal{G}_N \rightarrow \mathcal{H}^N$ is a continuous map.

(b) $\bullet : \mathcal{H} \times \mathcal{H} \rightarrow \mathcal{K}$ and $\otimes : \mathcal{H} \times \mathcal{H} \rightarrow \mathcal{L}$ are bilinear maps from $\mathcal{H} \times \mathcal{H}$ to two finite-dimensional (real) inner-product spaces $(\mathcal{K}, \langle \cdot, \cdot \rangle_{\mathcal{K}})$ and $(\mathcal{L}, \langle \cdot, \cdot \rangle_{\mathcal{L}})$, satisfying for all $\mathbf{a}, \mathbf{b}, \mathbf{a}', \mathbf{b}' \in \mathcal{H}$ the compatibility relation

$$\langle \mathbf{a} \bullet \mathbf{b}, \mathbf{a}' \bullet \mathbf{b}' \rangle_{\mathcal{K}} = \langle \mathbf{a} \otimes \mathbf{a}', \mathbf{b} \otimes \mathbf{b}' \rangle_{\mathcal{L}}. \quad (6)$$

(c) Let $B(\mathcal{H})$ be the space of linear operators on \mathcal{H} , and define an inclusion map $\iota : \mathcal{L} \rightarrow B(\mathcal{H})$ by

$$\langle \mathbf{a}, \iota(\mathbf{q})\mathbf{b} \rangle_{\mathcal{H}} = \langle \mathbf{q}, \mathbf{a} \otimes \mathbf{b} \rangle_{\mathcal{L}} \text{ for all } \mathbf{q} \in \mathcal{L} \text{ and } \mathbf{a}, \mathbf{b} \in \mathcal{H}. \quad (7)$$

Then ι is injective. Furthermore, corresponding to any element $\mathbf{q} \in \mathcal{L}$, there exist elements $|\mathbf{q}\rangle, |\mathbf{q}^\top\rangle \in \mathcal{L}$ such that $\iota(|\mathbf{q}\rangle), \iota(|\mathbf{q}^\top\rangle)$ are both symmetric positive-definite, and

$$\iota(|\mathbf{q}\rangle) = (\iota(\mathbf{q})^\top \iota(\mathbf{q}))^{1/2}, \quad \iota(|\mathbf{q}^\top\rangle) = (\iota(\mathbf{q})\iota(\mathbf{q}^\top))^{1/2}, \quad \|\mathbf{q}\|_{\mathcal{L}} = \||\mathbf{q}\rangle\|_{\mathcal{L}} = \||\mathbf{q}^\top\rangle\|_{\mathcal{L}}. \quad (8)$$

(d) Define an overlap map $Q : \mathcal{G}_N \times \mathcal{G}_N \rightarrow \mathcal{L}$ by

$$Q(G, H) = \frac{1}{N} \sum_{i=1}^N \phi(G)_i \otimes \phi(H)_i. \quad (9)$$

Then $Q(\cdot, \cdot)$ satisfies the group symmetry $Q(G, H) = Q(H^{-1}G, \text{Id})$ for any $G, H \in \mathcal{G}_N$, where Id is the identity element of \mathcal{G}_N .

¹We fix the noise standard deviation in (2) as \sqrt{N} without loss of generality, absorbing additional problem scalings into the definition of the N -dependent featurization ϕ .

We will illustrate how the group synchronization and quadratic assignment applications fit into this structure in Sections 3 and 4 to follow. For now, let us observe that under parts (b) and (d) of this assumption, applying the model definition (2), the Hamiltonian $H(G; Y)$ in (4) is approximately a linear combination of the squared overlaps

$$\begin{aligned} N\|Q(G, G)\|_{\mathcal{L}}^2 &= \frac{1}{N} \sum_{i,j=1}^N \langle \phi(G)_i \bullet \phi(G)_j, \phi(G)_i \bullet \phi(G)_j \rangle_{\mathcal{K}}, \\ N\|Q(G, G_*)\|_{\mathcal{L}}^2 &= \frac{1}{N} \sum_{i,j=1}^N \langle \phi(G)_i \bullet \phi(G)_j, \phi(G_*)_i \bullet \phi(G_*)_j \rangle_{\mathcal{K}}, \end{aligned}$$

and a \mathcal{G}_N -indexed centered Gaussian process $Z(G)$ with covariance kernel

$$\mathbb{E}[Z(G)Z(G')] = N\|Q(G, G')\|_{\mathcal{L}}^2 = \frac{1}{N} \sum_{i,j=1}^N \langle \phi(G)_i \bullet \phi(G)_j, \phi(G')_i \bullet \phi(G')_j \rangle_{\mathcal{K}}.$$

This structure mirrors that of the Bayes posterior law in low-rank matrix estimation problems. The error of this approximation for the Hamiltonian is² $O(K(\mathcal{G}_N))$ where

$$K(\mathcal{G}_N) = \sup_{G, G' \in \mathcal{G}_N} \frac{1}{N} \sum_{i=1}^N \|\phi(G)_i \otimes \phi(G')_i\|_{\mathcal{L}}^2 = \sup_{G, G' \in \mathcal{G}_N} \frac{1}{N} \sum_{i=1}^N \langle \phi(G)_i \bullet \phi(G)_i, \phi(G')_i \bullet \phi(G')_i \rangle_{\mathcal{K}}, \quad (10)$$

due to the removal of diagonal terms $i = j$ from the above squared overlap expressions. The group symmetry of $Q(\cdot, \cdot)$ in part (d) will ensure that the law over Y of the \mathcal{G}_N -valued process $\{H(G; Y)\}_{G \in \mathcal{G}_N}$ is, up to this $O(K(\mathcal{G}_N))$ discrepancy, independent of G_* . Finally, the inclusion map $\iota(\cdot)$ in part (c) identifies overlaps $\mathbf{q} \in \mathcal{L}$ with linear operators $\iota(\mathbf{q})$ on \mathcal{H} , and we will write the shorthands

$$\mathbf{q}\mathbf{a} := \iota(\mathbf{q})\mathbf{a}, \quad \mathbf{q}^{1/2}\mathbf{a} := \iota(\mathbf{q})^{1/2}\mathbf{a}, \quad (11)$$

the latter being well-defined when $\iota(\mathbf{q})$ is symmetric positive-semidefinite.

Under this assumption, the main result of this section is a general statement relating the free energy \mathcal{F}_N to the following model with linear observations of $\phi(G_*)$: Let

$$\mathcal{Q} = \left\{ \mathbf{q} \in \mathcal{L} : \iota(\mathbf{q}) \text{ is symmetric positive-semidefinite in } B(\mathcal{H}) \right\} \subset \mathcal{L}. \quad (12)$$

Fixing any $\mathbf{q} \in \mathcal{Q}$, consider the linear observation model with observations

$$\mathbf{y}_i = \mathbf{q}^{1/2}\phi(G_*)_i + \mathbf{z}_i \text{ for each } i = 1, \dots, N, \quad (13)$$

where $\mathbf{q}^{1/2}$ is identified as a linear operator on the feature space \mathcal{H} via (11), and $\{\mathbf{z}_i\}_{i=1}^N$ are i.i.d. standard Gaussian noise vectors in \mathcal{H} . Define a potential function $\Psi_N : \mathcal{Q} \rightarrow \mathbb{R}$ by

$$\Psi_N(\mathbf{q}) = -\frac{1}{4}\|\mathbf{q}\|_{\mathcal{L}}^2 - \frac{1}{2}\langle \mathbf{q}, Q(\text{Id}, \text{Id}) \rangle_{\mathcal{L}} + \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp \left(N\langle \mathbf{q}, Q(G, G_*) \rangle_{\mathcal{L}} + \sum_{i=1}^N \langle \mathbf{q}^{1/2}\phi(G)_i, \mathbf{z}_i \rangle_{\mathcal{H}} \right) \quad (14)$$

²Here and throughout, $O(f(N))$ denotes an error bounded in magnitude by $Cf(N)$ for an absolute constant $C > 0$.

where here \mathbb{E}_Z is the expectation over $Z = \{\mathbf{z}_i\}_{i=1}^N$. It is readily checked (c.f. Appendix A.4) that the signal-observation mutual information in the quadratic model (2) with observations $Y = (\mathbf{y}_{ij})_{i < j}$ is given by

$$\frac{1}{N} I(G_*, Y) := \frac{1}{N} \mathbb{E}_{G_*, Z} \log \frac{p(G_*, Y)}{p(G_*)p(Y)} = \frac{1}{4} \|Q(\text{Id}, \text{Id})\|_{\mathcal{L}}^2 - \mathcal{F}_N + O\left(\frac{K(\mathcal{G}_N)}{N}\right), \quad (15)$$

and the mutual information in the linear model (13) with observations $Y_{\text{lin}} = \{\mathbf{y}_i\}_{i=1}^N$ is given by

$$\frac{1}{N} i(G_*, Y_{\text{lin}}) = -\frac{1}{4} \|\mathbf{q}\|_{\mathcal{L}}^2 + \frac{1}{2} \langle \mathbf{q}, Q(\text{Id}, \text{Id}) \rangle_{\mathcal{L}} - \Psi_N(\mathbf{q}). \quad (16)$$

Our main result of this section is the following approximation of the free energy \mathcal{F}_N in terms of Ψ_N . This then provides a direct relation between the mutual informations $\frac{1}{N} I(G_*, Y)$ and $\frac{1}{N} i(G_*, Y_{\text{lin}})$ via (15) and (16), which we will spell out in the later applications of interest.

Theorem 2.2. *Denote*

$$\text{image}(Q) = \{Q(G, G') : G, G' \in \mathcal{G}_N\} \subset \mathcal{L},$$

let $D(\mathcal{G}_N) = \max\{\|\mathbf{q}\|_{\mathcal{L}} : \mathbf{q} \in \text{image}(Q)\}$, and let $L(\epsilon; \mathcal{G}_N)$ be the metric entropy of $\text{image}(Q)$, i.e. the log-cardinality of the smallest ϵ -cover of $\text{image}(Q)$ in the norm $\|\cdot\|_{\mathcal{L}}$. Under Assumption 2.1, there exists an absolute constant $C > 0$ such that for any $\epsilon > 0$,

$$\left| \mathcal{F}_N - \sup_{\mathbf{q} \in \mathcal{Q}} \Psi_N(\mathbf{q}) \right| \leq C \left(D(\mathcal{G}_N) \sqrt{\frac{L(\sqrt{\epsilon}; \mathcal{G}_N)}{N}} + \frac{K(\mathcal{G}_N) + L(\sqrt{\epsilon}; \mathcal{G}_N)}{N} + \epsilon \right).$$

Here, $K(\mathcal{G}_N)$, $D(\mathcal{G}_N)$, and $L(\sqrt{\epsilon}; \mathcal{G}_N)$ are finite by compactness of \mathcal{G}_N and continuity of ϕ , and these will all be of constant order for any fixed constant $\epsilon > 0$ in our applications to follow.

Overlap concentration. Denote by $\langle f(G) \rangle = \mathbb{E}[f(G) | Y]$ the posterior expectation given $Y = \{\mathbf{y}_{ij}\}_{i < j}$ in the quadratic model (2). An extension of our proof of Theorem 2.2 will establish that for G sampled from this posterior law, the overlap $Q(G, G_*)$ concentrates on a set defined by near-maximizers of the potential $\Psi_N(\mathbf{q})$. We give a general statement of this result here, and we will specialize this to a more interpretable statement in the group synchronization application of Section 3 to follow.

For any $A \in B(\mathcal{H})$, let p_A denote the marginal density of $Y_{\text{lin}} = \{\mathbf{y}_i\}_{i=1}^N$ in a linear observation model $\mathbf{y}_i = A\phi(G_*)_i + \mathbf{z}_i$ for $i = 1, \dots, N$, similar to (13). For $\mathbf{m} \in \mathcal{L}$ such that $\iota(\mathbf{m}) \in B(\mathcal{H})$ has singular value decomposition $\iota(\mathbf{m}) = UDV^\top$, denote

$$\mathbf{m}_U = D^{1/2}U^\top \in B(\mathcal{H}), \quad \mathbf{m}_V = D^{1/2}V^\top \in B(\mathcal{H}), \quad (17)$$

and recall from Assumption 2.1(c) that there exists $|\mathbf{m}| \in \mathcal{Q}$ for which $\iota(|\mathbf{m}|) = (\iota(\mathbf{m})^\top \iota(\mathbf{m}))^{1/2} = \mathbf{m}_V^\top \mathbf{m}_U$. Set³

$$\mathcal{L}_*(\epsilon) = \left\{ \mathbf{m} \in \mathcal{L} : \frac{1}{N} D_{\text{KL}}(p_{\mathbf{m}_V} \| p_{\mathbf{m}_U}) \leq \epsilon \text{ and } \sup_{\mathbf{q} \in \mathcal{Q}} \Psi_N(\mathbf{q}) - \Psi_N(|\mathbf{m}|) \leq \epsilon \right\}. \quad (18)$$

Intuitively, any $\mathbf{m} \in \mathcal{L}_*(\epsilon)$ is such that $|\mathbf{m}|$ is a near-maximizer of $\Psi_N(\cdot)$, and the condition $N^{-1} D_{\text{KL}}(p_{\mathbf{m}_V} \| p_{\mathbf{m}_U}) \approx 0$ captures a class of overlaps \mathbf{m} that are (nearly) equivalent to $|\mathbf{m}|$ under the group symmetry of the model.

³Here, for any $\mathbf{m} \in \mathcal{L}$, the element $|\mathbf{m}|$ is unique by the assumed injectivity of ι . It may also be checked that $D_{\text{KL}}(p_{\mathbf{m}_V} \| p_{\mathbf{m}_U})$ has the same value for any singular value decomposition UDV^\top of $\iota(\mathbf{m})$, so $\mathcal{L}_*(\epsilon)$ is well-defined.

Corollary 2.3. *In the setting of Theorem 2.2, there exist absolute constants $C_0, C, c > 0$ such that if*

$$\epsilon > C_0 \left(D(\mathcal{G}_N) \sqrt{\frac{L(\sqrt{\epsilon}; \mathcal{G}_N)}{N}} + \frac{K(\mathcal{G}_N) + L(\sqrt{\epsilon}; \mathcal{G}_N)}{N} \right) \quad (19)$$

then

$$\mathbb{E}_{G_*, Z} \left\langle \mathbf{1} \left\{ \|Q(G, G_*) - \mathcal{L}_*(\epsilon)\|_{\mathcal{L}}^2 > \epsilon \right\} \right\rangle \leq C \exp \left(-cN \min \left(\epsilon, \frac{\epsilon^2}{D(\mathcal{G}_N)^2} \right) \right) \quad (20)$$

where $\|Q(G, G_*) - \mathcal{L}_*(\epsilon)\|_{\mathcal{L}} := \inf \{ \|Q(G, G_*) - \mathbf{m}\| : \mathbf{m} \in \mathcal{L}_*(\epsilon) \}$.

The proofs of Theorem 2.2 and Corollary 2.3 are given in Appendix A. We prove both the lower and upper bounds for \mathcal{F}_N in Theorem 2.2 using an interpolation technique, the upper bound applying a method of [EAK18] to perform the interpolation on the Franz-Parisi potential at each fixed overlap. Corollary 2.3 then follows by applying similar arguments to bound a restriction of the free energy.

3 Group synchronization

As a first application of the results in Section 2, we consider a multi-channel group synchronization model, which is a real analogue of the model studied in [PWBM18]. Let \mathcal{G} be a compact group (fixed and not depending on N), and let $\phi_\ell : \mathcal{G} \rightarrow \mathbb{R}^{k_\ell \times k_\ell}$ for $\ell = 1, \dots, L$ be real orthogonal representations of \mathcal{G} . Throughout, corresponding to $\mathbf{g}, \mathbf{g}', \mathbf{g}_* \in \mathcal{G}$, we write the abbreviations

$$\mathbf{g}_\ell = \phi_\ell(\mathbf{g}), \quad \mathbf{g}'_\ell = \phi_\ell(\mathbf{g}'), \quad \mathbf{g}_{*\ell} = \phi_\ell(\mathbf{g}_*).$$

Let $G_* = (\mathbf{g}_*^{(1)}, \dots, \mathbf{g}_*^{(N)})$ be an unknown parameter vector of interest in the product space \mathcal{G}^N , with prior distribution $\{\mathbf{g}_*^{(i)}\}_{i=1}^N \stackrel{iid}{\sim} \text{Haar}(\mathcal{G})$.⁴ Consider the observations

$$\begin{cases} \mathbf{y}_1^{(ij)} = \sqrt{\lambda_1} \mathbf{g}_{*1}^{(i)} \mathbf{g}_{*1}^{(j)\top} + \sqrt{N} \mathbf{z}_1^{(ij)} \in \mathbb{R}^{k_1 \times k_1} \\ \vdots \\ \mathbf{y}_L^{(ij)} = \sqrt{\lambda_L} \mathbf{g}_{*L}^{(i)} \mathbf{g}_{*L}^{(j)\top} + \sqrt{N} \mathbf{z}_L^{(ij)} \in \mathbb{R}^{k_L \times k_L} \end{cases} \quad \text{for all } 1 \leq i < j \leq N \quad (21)$$

where $\lambda_\ell > 0$ are fixed and known signal-to-noise parameters, and $\{\mathbf{z}_\ell^{(ij)}\}_{1 \leq i < j \leq N, 1 \leq \ell \leq L}$ are noise matrices with i.i.d. $\mathcal{N}(0, 1)$ entries, independent of each other and of G_* .

We note that any observation model (21) is equivalent to such a model in a ‘‘canonical’’ form where the representations ϕ_1, \dots, ϕ_L are real-irreducible, distinct, and non-trivial; this canonical form may be a multi-channel model even if the original problem consists of a single channel $L = 1$. We explain this reduction in Appendix D.3, where we also review some relevant background and terminology pertaining to group representations.

This model falls into the general framework described in Section 2. Here, $\mathcal{G}_N \equiv \mathcal{G}^N$ is the N -fold product of \mathcal{G} . For $G = (\mathbf{g}^{(1)}, \dots, \mathbf{g}^{(N)}) \in \mathcal{G}_N$, the feature map $\phi : \mathcal{G}_N \rightarrow \mathcal{H}^N$ is separable across coordinates $i = 1, \dots, N$, with components

$$\phi(G)_i = (\mathbf{g}_1^{(i)}, \dots, \mathbf{g}_L^{(i)}) \in \mathcal{H} \equiv \prod_{\ell=1}^L \mathbb{R}^{k_\ell \times k_\ell}. \quad (22)$$

⁴For simplicity of the later notation, in this group synchronization model we will use superscripts for the sample index $i \in [N]$ and subscripts for the channel index $\ell \in [L]$.

We identify the observation and overlap spaces also as $\mathcal{K} = \mathcal{L} = \mathcal{H} = \prod_{\ell=1}^L \mathbb{R}^{k_\ell \times k_\ell}$, equipped with the usual Euclidean inner-products

$$\langle \mathbf{a}, \mathbf{b} \rangle_{\mathcal{H}} = \langle \mathbf{a}, \mathbf{b} \rangle_{\mathcal{K}} = \langle \mathbf{a}, \mathbf{b} \rangle_{\mathcal{L}} = \sum_{\ell=1}^L \text{Tr} \mathbf{a}_\ell^\top \mathbf{b}_\ell.$$

The pair of bilinear maps $\bullet : \mathcal{H} \times \mathcal{H} \rightarrow \mathcal{K}$ and $\otimes : \mathcal{H} \times \mathcal{H} \rightarrow \mathcal{L}$ and the inclusion map $\iota : \mathcal{L} \rightarrow B(\mathcal{H})$ are then defined as

$$\mathbf{a} \bullet \mathbf{b} = \left(\sqrt{\lambda_\ell} \mathbf{a}_\ell \mathbf{b}_\ell^\top \right)_{\ell=1}^L, \quad \mathbf{a} \otimes \mathbf{b} = \left(\sqrt{\lambda_\ell} \mathbf{a}_\ell^\top \mathbf{b}_\ell \right)_{\ell=1}^L, \quad \iota(\mathbf{q})\mathbf{a} = \left(\sqrt{\lambda_\ell} \mathbf{a}_\ell \mathbf{q}_\ell^\top \right)_{\ell=1}^L. \quad (23)$$

We will check in the proof of Theorem 3.1 below that the structure of Assumption 2.1 indeed holds under these definitions.

We write $\text{Sym}^{k \times k}$, $\text{Sym}_{\geq 0}^{k \times k}$ for the spaces of $k \times k$ symmetric and symmetric-positive-semidefinite matrices, respectively, and abbreviate

$$\text{Sym} = \prod_{\ell=1}^L \text{Sym}^{k_\ell \times k_\ell}, \quad \text{Sym}_{\geq 0} = \prod_{\ell=1}^L \text{Sym}_{\geq 0}^{k_\ell \times k_\ell},$$

$$\mathbf{g}\mathbf{q}\mathbf{g}' = \left(\mathbf{g}_\ell \mathbf{q}_\ell \mathbf{g}'_\ell \right)_{\ell=1}^L \in \mathcal{L} \quad \text{for any } \mathbf{g}, \mathbf{g}' \in \mathcal{G} \text{ and } \mathbf{q} \in \text{Sym}.$$

3.1 Asymptotic mutual information and MMSE

Let $Y = \{\mathbf{y}_\ell^{(ij)}\}$ be the collection of all observations, and let $\langle f(G) \rangle = \langle f(\mathbf{g}^{(1)}, \dots, \mathbf{g}^{(N)}) \rangle$ denote the average under the posterior law of $G = (\mathbf{g}^{(1)}, \dots, \mathbf{g}^{(N)}) \in \mathcal{G}^N$ given Y . Let $I(G_*, Y)$ be the mutual information between $G_* = (\mathbf{g}_*^{(1)}, \dots, \mathbf{g}_*^{(N)})$ and Y , and let

$$\text{MMSE}_\ell = \frac{1}{\binom{N}{2}} \sum_{1 \leq i < j \leq N} \mathbb{E} \|\mathbf{g}_{*\ell}^{(i)\top} \mathbf{g}_{*\ell}^{(j)} - \langle \mathbf{g}_\ell^{(i)\top} \mathbf{g}_\ell^{(j)} \rangle\|_F^2 \quad \text{for each } \ell = 1, \dots, L \quad (24)$$

be the Bayes-optimal minimum mean-squared-error (MMSE) for estimating $\{\mathbf{g}_{*\ell}^{(i)\top} \mathbf{g}_{*\ell}^{(j)}\}_{1 \leq i < j \leq N}$ in the ℓ^{th} channel.

Define the replica potential $\Psi_{\text{gs}} : \text{Sym}_{\geq 0} \rightarrow \mathbb{R}$ by

$$\Psi_{\text{gs}}(\mathbf{q}) = -\frac{1}{4} \sum_{\ell=1}^L \lambda_\ell \|\mathbf{q}_\ell\|_F^2 - \frac{1}{2} \sum_{\ell=1}^L \lambda_\ell \text{Tr} \mathbf{q}_\ell + \mathbb{E}_{\mathbf{g}_*, \mathbf{z}} \log \mathbb{E}_{\mathbf{g}} \exp \left(\sum_{\ell=1}^L \lambda_\ell \text{Tr} \mathbf{q}_\ell \mathbf{g}_\ell^\top \mathbf{g}_{*\ell} + \sqrt{\lambda_\ell} \text{Tr} \mathbf{q}_\ell^{1/2} \mathbf{g}_\ell^\top \mathbf{z}_\ell \right) \quad (25)$$

where $\mathbb{E}_{\mathbf{g}}$ is the expectation over a single uniformly distributed group element $\mathbf{g} \sim \text{Haar}(\mathcal{G})$, and $\mathbb{E}_{\mathbf{g}_*, \mathbf{z}}$ is over an independent element $\mathbf{g}_* \sim \text{Haar}(\mathcal{G})$ and Gaussian noise $\mathbf{z} = (\mathbf{z}_1, \dots, \mathbf{z}_L) \in \prod_{\ell=1}^L \mathbb{R}^{k_\ell \times k_\ell}$ with i.i.d. $\mathcal{N}(0, 1)$ entries. By invariance of Haar measure and invariance in law of each \mathbf{z}_ℓ under multiplication by orthogonal matrices, it may be checked that Ψ_{gs} has the group symmetry

$$\Psi_{\text{gs}}(\mathbf{q}) = \Psi_{\text{gs}}(\mathbf{g}\mathbf{q}\mathbf{g}^{-1}) \text{ for all } \mathbf{g}, \mathbf{g}' \in \mathcal{G} \text{ and } \mathbf{q} \in \text{Sym}_{\geq 0}. \quad (26)$$

In particular, the set of maximizers of Ψ_{gs} is closed under the mapping $\mathbf{q} \mapsto \mathbf{g}\mathbf{q}\mathbf{g}^{-1}$ for all $\mathbf{g} \in \mathcal{G}$. It is also direct to check, similarly to (16), that Ψ_{gs} satisfies

$$i(\mathbf{g}_*, \mathbf{y}) = \sum_{\ell=1}^L \left(-\frac{\lambda_\ell}{4} \|\mathbf{q}_\ell\|_F^2 + \frac{\lambda_\ell}{2} \text{Tr} \mathbf{q}_\ell \right) - \Psi_{\text{gs}}(\mathbf{q}) \quad (27)$$

where $i(\mathbf{g}_*, \mathbf{y})$ is the mutual information between the signal $\mathbf{g}_* \in \mathcal{G}$ and observations $\mathbf{y} = (\mathbf{y}_1, \dots, \mathbf{y}_L)$ in a \mathbf{q} -dependent “single-sample” model

$$\begin{cases} \mathbf{y}_1 = \sqrt{\lambda_1} \mathbf{g}_{*1} \mathbf{q}_1^{1/2} + \mathbf{z}_1 \in \mathbb{R}^{k_1 \times k_1} \\ \vdots \\ \mathbf{y}_L = \sqrt{\lambda_L} \mathbf{g}_{*L} \mathbf{q}_L^{1/2} + \mathbf{z}_L \in \mathbb{R}^{k_L \times k_L}. \end{cases} \quad (28)$$

The following is an application of Theorem 2.2 and Corollary 2.3, characterizing the asymptotic mutual information, per-channel MMSE, and concentration of the posterior overlap with the true signal in this group synchronization model as $N \rightarrow \infty$, in terms of a maximization of the above replica potential.

Theorem 3.1. *Suppose the group \mathcal{G} , representations ϕ_1, \dots, ϕ_L , and signal strengths $\lambda_1, \dots, \lambda_L > 0$ are fixed, as $N \rightarrow \infty$.*

(a) *The signal-observation mutual information $I(G_*, Y)$ in the model (21) satisfies*

$$\lim_{N \rightarrow \infty} \frac{1}{N} I(G_*, Y) = \frac{1}{4} \sum_{\ell=1}^L \lambda_\ell k_\ell - \sup_{\mathbf{q} \in \text{Sym}_{\geq 0}} \Psi_{\text{gs}}(\mathbf{q}). \quad (29)$$

(b) *Fixing any $\ell \in \{1, \dots, L\}$ and positive values $\{\lambda'_\ell\}_{\ell' \neq \ell}$, set*

$$D = \left\{ \lambda_\ell > 0 : \lambda_\ell \mapsto \sup_{\mathbf{q} \in \text{Sym}_{\geq 0}} \Psi_{\text{gs}}(\mathbf{q}) \text{ is differentiable at } \lambda_\ell \right\}.$$

Then D has full Lebesgue measure in $(0, \infty)$. We have $\lambda_\ell \in D$ if and only if all maximizers \mathbf{q}_ of $\Psi_{\text{gs}}(\mathbf{q})$ have the same ℓ -th component Frobenius norm $\|\mathbf{q}_{*\ell}\|_F$, in which case*

$$\lim_{N \rightarrow \infty} \text{MMSE}_\ell = k_\ell - \|\mathbf{q}_{*\ell}\|_F^2. \quad (30)$$

(c) *Denote*

$$\mathcal{L}_{*, \text{gs}} = \left\{ \mathbf{g} \mathbf{q}_* : \mathbf{q}_* \in \arg \max_{\mathbf{q} \in \text{Sym}_{\geq 0}} \Psi_{\text{gs}}(\mathbf{q}) \text{ and } \mathbf{g} \in \mathcal{G} \right\} \subset \mathcal{L} \quad (31)$$

and define a neighborhood $\mathcal{L}_{, \text{gs}}(\epsilon) = \{\mathbf{m} \in \mathcal{L} : \inf_{\mathbf{m}_* \in \mathcal{L}_{*, \text{gs}}} \sum_{\ell=1}^L \lambda_\ell \|\mathbf{m}_\ell - \mathbf{m}_{*\ell}\|_F^2 < \epsilon\}$. Then for any $\epsilon > 0$, there exist constants $C, c > 0$ depending only on $\mathcal{G}, \phi_1, \dots, \phi_L, \epsilon$ such that*

$$\mathbb{E} \left\langle \mathbf{1} \left\{ \left(\frac{1}{N} \sum_{i=1}^N \mathbf{g}_\ell^{(i)\top} \mathbf{g}_{*\ell}^{(i)} \right)_{\ell=1}^L \notin \mathcal{L}_{*, \text{gs}}(\epsilon) \right\} \right\rangle \leq C e^{-cN}.$$

We remark that the parameter $G_* = (\mathbf{g}_*^{(1)}, \dots, \mathbf{g}_*^{(N)})$ in this model is identifiable only up to a global rotation $(\mathbf{g}_*^{(1)}, \dots, \mathbf{g}_*^{(N)}) \mapsto (\mathbf{g}_*^{(1)} \mathbf{g}, \dots, \mathbf{g}_*^{(N)} \mathbf{g})$ by any single group element $\mathbf{g} \in \mathcal{G}$, and the posterior law is invariant under this transformation. The above set $\mathcal{L}_{*, \text{gs}}$ may be understood as the set of overlaps that are equivalent to a global maximizer of Ψ_{gs} up to this group invariance of the posterior law, and part (c) of this theorem shows that the overlap of a posterior sample G with the true signal G_* concentrates near this set $\mathcal{L}_{*, \text{gs}}$ in the $N \rightarrow \infty$ limit.

3.2 Critical points and algorithmic phase transition

Theorem 3.1 implies that the signal-observation mutual information and information-theoretic MMSE are governed by the global maximizer(s) of the replica potential Ψ_{gs} .

In contrast, the local optimality of $\mathbf{q} = \mathbf{0}$ is conjectured to govern the feasibility of computationally-efficient weak signal recovery (i.e. of attaining non-zero asymptotic overlap $\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N \widehat{\mathbf{g}}_\ell^{(i)\top} \widehat{\mathbf{g}}_{*\ell}^{(i)}$ for some channel $\ell \in \{1, \dots, L\}$ by a polynomial-time estimator $\widehat{\mathbf{g}}$). In particular, Approximate Message Passing (AMP) algorithms of the form developed in [PWBM18] are expected to achieve weak signal recovery from a random initialization whenever $\mathbf{q} = \mathbf{0}$ is *not* a local maximizer of Ψ_{gs} , and conversely it is conjectured that no polynomial-time algorithm can achieve weak signal recovery when $\mathbf{q} = \mathbf{0}$ is a local maximizer of Ψ_{gs} . We refer to [LKZ17, LM19] for discussion of this conjecture in related low-rank matrix estimation problems.

In this section, for general synchronization problems, we provide a criterion for the local optimality of $\mathbf{q} = \mathbf{0}$ for maximizing Ψ_{gs} , in terms of the signal strengths and classifications of the real-irreducible components of the observation channels.

The following proposition first derives general forms for the gradient and Hessian of Ψ_{gs} . We write $\nabla \Psi_{\text{gs}}(\mathbf{q})$ and $\nabla^2 \Psi_{\text{gs}}(\mathbf{q})$ for this gradient and Hessian as linear and bilinear forms on Sym . When \mathbf{q} is in the strict interior of $\text{Sym}_{\geq 0}$, these are defined by the Taylor expansion

$$\Psi_{\text{gs}}(\mathbf{q} + \mathbf{x}) = \Psi_{\text{gs}}(\mathbf{q}) + \nabla \Psi_{\text{gs}}(\mathbf{q})[\mathbf{x}] + \frac{1}{2} \nabla^2 \Psi_{\text{gs}}(\mathbf{q})[\mathbf{x}, \mathbf{x}] + o(\|\mathbf{x}\|^2) \quad \text{for } \mathbf{x} \in \text{Sym} \text{ with } \|\mathbf{x}\| \rightarrow 0,$$

and we extend these definitions of $\nabla \Psi_{\text{gs}}$ and $\nabla^2 \Psi_{\text{gs}}$ by continuity to the boundary of $\text{Sym}_{\geq 0}$.

Proposition 3.2. *Let $\langle f(\mathbf{g}) \rangle_{\mathbf{q}}$ be the mean under the posterior law of \mathbf{g} in the single-sample model (28).*

(a) *For any $\mathbf{q} = (\mathbf{q}_1, \dots, \mathbf{q}_L) \in \text{Sym}_{\geq 0}$ and $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_L) \in \text{Sym}$,*

$$\nabla \Psi_{\text{gs}}(\mathbf{q})[\mathbf{x}] = \sum_{\ell=1}^L -\frac{\lambda_\ell}{2} \text{Tr } \mathbf{x}_\ell \left(\mathbf{q}_\ell - \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \mathbf{g}_{*\ell}^\top \langle \mathbf{g}_\ell \rangle_{\mathbf{q}} \right) = \sum_{\ell=1}^L -\frac{\lambda_\ell}{2} \text{Tr } \mathbf{x}_\ell \left(\mathbf{q}_\ell - \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \langle \mathbf{g}_\ell \rangle_{\mathbf{q}}^\top \langle \mathbf{g}_\ell \rangle_{\mathbf{q}} \right). \quad (32)$$

*In particular, $\nabla \Psi_{\text{gs}}(\mathbf{q}) = 0$ if and only if $\mathbf{q}_\ell = \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \langle \mathbf{g}_\ell \rangle_{\mathbf{q}}^\top \langle \mathbf{g}_\ell \rangle_{\mathbf{q}}$ for every $\ell = 1, \dots, L$.*

(b) *For any $\mathbf{q} = (\mathbf{q}_1, \dots, \mathbf{q}_L) \in \text{Sym}_{\geq 0}$, $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_L) \in \text{Sym}$, and $\mathbf{x}' = (\mathbf{x}'_1, \dots, \mathbf{x}'_L) \in \text{Sym}$,*

$$\begin{aligned} \nabla^2 \Psi_{\text{gs}}(\mathbf{q})[\mathbf{x}, \mathbf{x}'] &= \sum_{\ell=1}^L -\frac{\lambda_\ell}{2} \text{Tr } \mathbf{x}_\ell \mathbf{x}'_\ell + \sum_{\ell, \ell'=1}^L \frac{\lambda_\ell \lambda_{\ell'}}{2} \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \left[\left\langle \text{Tr } \mathbf{x}_\ell \mathbf{g}_{*\ell}^\top \mathbf{g}_\ell \text{ Tr } \mathbf{x}'_{\ell'} \mathbf{g}_{*\ell'}^\top \mathbf{g}_{\ell'} \right\rangle_{\mathbf{q}} \right. \\ &\quad \left. - 2 \text{Tr } \mathbf{x}_\ell \mathbf{g}_{*\ell}^\top \langle \mathbf{g}_\ell \rangle_{\mathbf{q}} \text{ Tr } \mathbf{x}'_{\ell'} \mathbf{g}_{*\ell'}^\top \langle \mathbf{g}_{\ell'} \rangle_{\mathbf{q}} + \text{Tr } \mathbf{x}_\ell \langle \mathbf{g}_\ell \rangle_{\mathbf{q}}^\top \langle \mathbf{g}_\ell \rangle_{\mathbf{q}} \text{ Tr } \mathbf{x}'_{\ell'} \langle \mathbf{g}_{\ell'} \rangle_{\mathbf{q}}^\top \langle \mathbf{g}_{\ell'} \rangle_{\mathbf{q}} \right]. \end{aligned} \quad (33)$$

If a representation $\mathbf{g}_\ell = \phi_\ell(\mathbf{g})$ is *not* real-irreducible, then applying an orthogonal change-of-basis so that the matrices $\{\phi_\ell(\mathbf{g}) : \mathbf{g} \in \mathcal{G}\}$ are simultaneously block-diagonal (c.f. Theorem D.12), part (a) of this proposition implies that $\nabla \Psi_{\text{gs}}(\mathbf{q}) = 0$ can only hold when \mathbf{q}_ℓ has this same block-diagonal structure. Maximization of $\Psi_{\text{gs}}(\mathbf{q})$ may then be restricted to \mathbf{q}_ℓ having this structure, in agreement with the reduction in Appendix D.3 of the model (21) to a canonical form having only real-irreducible representations.

Assuming such a canonical form, the next result characterizes the phase transition threshold for $\mathbf{q} = \mathbf{0}$ to locally maximize $\Psi_{\text{gs}}(\mathbf{q})$. We recall in Appendix D.2 that any real-irreducible representation ϕ_ℓ can be categorized as being of “real type” if ϕ_ℓ is also \mathbb{C} -irreducible, of “complex type” if $\phi_\ell \cong \psi \oplus \bar{\psi}$ where $\psi, \bar{\psi}$ are \mathbb{C} -irreducible complex-conjugate sub-representations with $\psi \not\cong \bar{\psi}$, or of “quaternionic type” if $\phi_\ell \cong \psi \oplus \psi$ where ψ is \mathbb{C} -irreducible and $\psi \cong \bar{\psi}$; the type of ϕ_ℓ may be determined from the value of $\rho_\ell := \mathbb{E}_{\mathbf{g}}[(\text{Tr } \mathbf{g}_\ell)^2]$.

Proposition 3.3. *Suppose ϕ_1, \dots, ϕ_L are real-irreducible, distinct, and non-trivial representations of \mathcal{G} . Let*

$$\rho_\ell := \mathbb{E}_{\mathbf{g}}[(\text{Tr } \mathbf{g}_\ell)^2] = \begin{cases} 1 & \text{if } \mathbf{g}_\ell \text{ is of real type} \\ 2 & \text{if } \mathbf{g}_\ell \text{ is of complex type} \\ 4 & \text{if } \mathbf{g}_\ell \text{ is of quaternionic type} \end{cases} \quad (34)$$

and set $\tilde{\lambda}_\ell = \lambda_\ell \rho_\ell / k_\ell$. Then at $\mathbf{q} = \mathbf{0}$, we have $\nabla \Psi_{\text{gs}}(\mathbf{0}) = 0$. Furthermore,

- (a) If $\max_{\ell=1}^L \tilde{\lambda}_\ell < 1$, then $\nabla^2 \Psi_{\text{gs}}(\mathbf{0})$ is negative-definite, and $\mathbf{q} = \mathbf{0}$ is a local maximizer of $\Psi_{\text{gs}}(\mathbf{q})$.
(b) If $\max_{\ell=1}^L \tilde{\lambda}_\ell > 1$, then $\nabla^2 \Psi_{\text{gs}}(\mathbf{0})$ has a positive eigenvalue, and $\mathbf{q} = \mathbf{0}$ is not a local maximizer of $\Psi_{\text{gs}}(\mathbf{q})$.

Let us spell out the implication of this result for four specific examples of synchronization problems over rotation and permutation groups, due to their particular interest in applications [Sin11, PKS13, BCLS20].

Example 3.4 (Multi-channel angular synchronization). Let

$$\mathcal{G} = \mathbb{S}\mathbb{O}(2) = \left\{ \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} : \theta \in [0, 2\pi) \right\}. \quad (35)$$

Identifying $\mathbf{g} \in \mathcal{G}$ with its rotation angle $\theta \in [0, 2\pi)$, consider the multi-channel observation model (21) with the representations

$$\mathbf{g}_\ell = \begin{pmatrix} \cos \ell\theta & -\sin \ell\theta \\ \sin \ell\theta & \cos \ell\theta \end{pmatrix} \in \mathbb{R}^{2 \times 2} \text{ for } \ell = 1, \dots, L. \quad (36)$$

(The setting of single-channel angular synchronization corresponds to $L = 1$.)

Here, the representations \mathbf{g}_ℓ are distinct, and each representation \mathbf{g}_ℓ is real-irreducible: Indeed, for any two unit vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^2$ there exists $\theta \in [0, 2\pi)$ for which \mathbf{g}_ℓ defined by (36) satisfies $\mathbf{u} = \mathbf{g}_\ell \mathbf{v}$, so no subspace of \mathbb{R}^2 is invariant. We have $\mathbb{E}[(\text{Tr } \mathbf{g}_\ell)^2] = \mathbb{E}_{\theta \sim \text{Unif}([0, 2\pi))}[(2 \cos \ell\theta)^2] = 2$, so each representation \mathbf{g}_ℓ is of complex type.

Then Proposition 3.3 implies that $\mathbf{q} = \mathbf{0}$ is a local maximizer of Ψ_{gs} if $\max_{\ell=1}^L \lambda_\ell < 1$, and it is not a local maximizer if $\max_{\ell=1}^L \lambda_\ell > 1$.

Example 3.5 (Rotational synchronization). Let $\mathcal{G} = \mathbb{S}\mathbb{O}(k)$, and consider a single-channel model with the standard representation $\phi(\mathbf{g}) = \mathbf{g} \in \mathbb{R}^{k \times k}$ given by its rotational action on \mathbb{R}^k . That is, for an unknown signal vector $G_* = (\mathbf{g}_*^{(1)}, \dots, \mathbf{g}_*^{(N)})$ with prior distribution $\{\mathbf{g}_*^{(i)}\}_{i=1}^N \stackrel{iid}{\sim} \text{Haar}(\mathbb{S}\mathbb{O}(k))$, we observe

$$\mathbf{y}^{(ij)} = \sqrt{\lambda} \mathbf{g}_*^{(i)\top} \mathbf{g}_*^{(j)} + \sqrt{N} \mathbf{z}^{(ij)} \in \mathbb{R}^{k \times k} \quad \text{for } 1 \leq i < j \leq N$$

where $\mathbf{z}^{(ij)}$ are independent noise matrices with i.i.d. $\mathcal{N}(0, 1)$ entries.

This representation is real-irreducible, for the same reason as in Example 3.4. For $k = 2$, it is of complex type as shown in Example 3.4. For $k \geq 3$, we have $\mathbb{E}[g_{ii}g_{jj}] = 0$ for all $i \neq j$ and $\mathbb{E}[g_{ij}^2] = \frac{1}{k^2} \mathbb{E} \text{Tr } \mathbf{g}^\top \mathbf{g} = \frac{1}{k}$ for all $i, j \in \{1, \dots, k\}$, by the invariances in law of $\mathbb{S}\mathbb{O}(k)$ under negations and transpositions of rows and columns. Thus $\mathbb{E}[(\text{Tr } \mathbf{g})^2] = \mathbb{E}[\sum_{i=1}^k g_{ii}^2] = 1$, so the representation is of real type (i.e. it is also \mathbb{C} -irreducible).

Set

$$\lambda_c := \begin{cases} 1 & \text{if } k = 2 \\ k & \text{if } k \geq 3. \end{cases}$$

Proposition 3.3 then implies that $\mathbf{q} = \mathbf{0}$ is a local maximizer of Ψ_{gs} for $\lambda < \lambda_c$, and it is not a local maximizer for $\lambda > \lambda_c$.

Example 3.6 (Cyclic permutation synchronization). Let $\mathcal{G} = \mathbb{Z}/k\mathbb{Z}$ be the cyclic group of size k , with elements $\{\text{Id}, \mathbf{h}, \mathbf{h}^2, \dots, \mathbf{h}^{k-1}\}$, and consider its action on \mathbb{R}^k by cyclic permutations of coordinates. We note that the span of $\mathbf{e} = (1, 1, \dots, 1) \in \mathbb{R}^k$ is a trivial invariant subspace of this action, which carries no information about the permutation. Hence, let us consider the model defined by $\phi(\mathbf{g}) \in \mathbb{R}^{(k-1) \times (k-1)}$ representing the restriction of this action to the subspace orthogonal to \mathbf{e} , under any choice of orthonormal basis for this subspace. That is, for an unknown signal vector $G_* = (\mathbf{g}_*^{(1)}, \dots, \mathbf{g}_*^{(N)})$ with prior distribution $\{\mathbf{g}_*^{(i)}\}_{i=1}^N \stackrel{iid}{\sim} \text{Haar}(\mathbb{Z}/k\mathbb{Z})$, we observe

$$\mathbf{y}^{(ij)} = \sqrt{\lambda} \phi(\mathbf{g}_*^{(i)})^\top \phi(\mathbf{g}_*^{(j)}) + \sqrt{N} \mathbf{z}^{(ij)} \in \mathbb{R}^{(k-1) \times (k-1)} \quad \text{for } 1 \leq i < j \leq N$$

where $\mathbf{z}^{(ij)}$ are again independent noise matrices with i.i.d. $\mathcal{N}(0, 1)$ entries.

Suppose (for simplicity of discussion) that $k \geq 3$ is odd. Then $\{\phi(\mathbf{g}) : \mathbf{g} \in \mathbb{Z}/k\mathbb{Z}\}$ leaves invariant the 2-dimensional subspaces $\{S_\ell\}_{\ell=1}^{(k-1)/2}$ of \mathbb{R}^k orthogonal to \mathbf{e} , spanned by the pairs of vectors

$$\left(1, \cos \frac{2\pi\ell}{k}, \cos \frac{4\pi\ell}{k}, \dots, \cos \frac{2\pi\ell(k-1)}{k}\right), \quad \left(0, \sin \frac{2\pi\ell}{k}, \sin \frac{4\pi\ell}{k}, \dots, \sin \frac{2\pi\ell(k-1)}{k}\right).$$

The sub-representation of $\phi(\cdot)$ restricted to each subspace S_ℓ is isomorphic to the representation given by

$$\phi_\ell(\mathbf{h}^j) = \begin{pmatrix} \cos(2\pi\ell j/k) & -\sin(2\pi\ell j/k) \\ \sin(2\pi\ell j/k) & \cos(2\pi\ell j/k) \end{pmatrix} \in \mathbb{R}^{2 \times 2},$$

so (c.f. Appendix D.3) this model is equivalent to a multi-channel model in which we observe

$$\mathbf{y}_\ell^{(ij)} = \sqrt{\lambda} \mathbf{g}_{*\ell}^{(i)\top} \mathbf{g}_{*\ell}^{(j)} + \sqrt{N} \mathbf{z}_\ell^{(ij)} \in \mathbb{R}^{2 \times 2}$$

for all $\ell = 1, \dots, (k-1)/2$ and $1 \leq i < j \leq N$, with $\mathbf{g}_{*\ell}^{(i)} = \phi_\ell(\mathbf{g}_*^{(i)})$. These representations ϕ_ℓ are distinct, real-irreducible, and of complex type by a similar argument as in Example 3.4.

Thus, Proposition 3.3 shows that $\mathbf{q} = \mathbf{0}$ is a local maximizer of Ψ_{gs} if $\lambda < 1$, and it is not a local maximizer if $\lambda > 1$.

Example 3.7 (Permutation synchronization). Consider now the full symmetric group $\mathcal{G} = \mathbb{S}_k$, with action by permutation of coordinates on \mathbb{R}^k . Again, as $\mathbf{e} = (1, 1, \dots, 1) \in \mathbb{R}^k$ spans a trivial invariant subspace, we consider the model defined by the standard representation $\phi(\mathbf{g}) \in \mathbb{R}^{(k-1) \times (k-1)}$ representing this action on the subspace orthogonal to \mathbf{e} . That is, for an unknown signal vector $G_* = (\mathbf{g}_*^{(1)}, \dots, \mathbf{g}_*^{(N)})$ with prior distribution $\{\mathbf{g}_*^{(i)}\}_{i=1}^N \stackrel{iid}{\sim} \text{Haar}(\mathbb{S}_k)$, we observe

$$\mathbf{y}^{(ij)} = \sqrt{\lambda} \phi(\mathbf{g}_*^{(i)})^\top \phi(\mathbf{g}_*^{(j)}) + \sqrt{N} \mathbf{z}^{(ij)} \in \mathbb{R}^{(k-1) \times (k-1)} \quad \text{for } 1 \leq i < j \leq N$$

where $\mathbf{z}^{(ij)}$ are again independent noise matrices with i.i.d. $\mathcal{N}(0, 1)$ entries. Here, the standard representation $\phi(\cdot)$ is \mathbb{C} -irreducible [FH13, Proposition 3.12], and hence also real-irreducible of real type.

Thus, Proposition 3.3 shows that $\mathbf{q} = \mathbf{0}$ is a local maximizer of Ψ_{gs} if $\lambda < k-1$, and it is not a local maximizer if $\lambda > k-1$.

More generally, the algorithmic phase transition threshold for local optimality of $\mathbf{q} = \mathbf{0}$ in any such example may be deduced by first reducing the model to a canonical form as described in Appendix D.3, then determining the type of each real-irreducible component, and finally determining the thresholds for their corresponding signal strengths from Proposition 3.3.

Remark 3.8. The work [PWBM18] studied a version of this model of the form

$$\begin{cases} \mathbf{y}_1^{(ij)} = \sqrt{\lambda_1} \mathbf{g}_{*1}^{(i)} \mathbf{g}_{*1}^{(j)*} + \sqrt{N} \mathbf{z}_1^{(ij)} \in \mathbb{C}^{k_1 \times k_1} \\ \vdots \\ \mathbf{y}_L^{(ij)} = \sqrt{\lambda_L} \mathbf{g}_{*L}^{(i)} \mathbf{g}_{*L}^{(j)*} + \sqrt{N} \mathbf{z}_L^{(ij)} \in \mathbb{C}^{k_L \times k_L} \end{cases} \quad \text{for all } 1 \leq i < j \leq N \quad (37)$$

where $\mathbf{g}_{*\ell} = \phi_\ell(\mathbf{g}_*) \in \mathbb{C}^{k_\ell \times k_\ell}$ for $\ell = 1, \dots, L$ correspond to distinct \mathbb{C} -irreducible representations of \mathcal{G} , and $\{\mathbf{z}_\ell^{(ij)}\}_{i < j}$ are the sub-blocks of $k_\ell N \times k_\ell N$ noise matrices distributed according to the GOE, GUE, or GSE depending on the type of the representation ϕ_ℓ . For such a model, [PWBM18] developed and analyzed an AMP algorithm for Bayes-optimal inference, and stated also a replica formula for the free energy that is similar to (25). It was argued (more heuristically) in [PWBM18, Section 6.6] that $\mathbf{q} = \mathbf{0}$ is a stable fixed point of this AMP algorithm if and only if $\max_{\ell=1}^L \lambda_\ell/k_\ell < 1$. Our results of Theorem 3.1 and Proposition 3.3 thus provide rigorous proofs of analogous statements in a real version of this model.

One difference between our analyses and those of [PWBM18]—in addition to the real vs. complex distinction—is that the replica formula stated in [PWBM18] implicitly assumes that the maximization of $\Psi_{\text{gs}}(\mathbf{q})$ may be restricted to overlaps $\mathbf{q} = (\mathbf{q}_1, \dots, \mathbf{q}_L)$ where each \mathbf{q}_ℓ is a scalar multiple of the identity matrix. The analyses of AMP state evolution in [PWBM18] also assume an initialization at overlaps \mathbf{q} of this form, and stability of the state evolution at $\mathbf{q} = \mathbf{0}$ is analyzed under this restriction of \mathbf{q} . Outside the setting of abelian groups (c.f. Proposition 3.9 below), we have not found a general argument that $\Psi_{\text{gs}}(\mathbf{q})$ must always be maximized at a point where each \mathbf{q}_ℓ is a multiple of the identity; furthermore, one typically may not have an initialization for AMP that corresponds to this type of initial state. We have thus defined the replica potential Ψ_{gs} over all symmetric positive-semidefinite overlaps \mathbf{q} , and our result of Proposition 3.3 pertains to the local optimality of $\mathbf{q} = \mathbf{0}$ with respect to optimization of Ψ_{gs} over this full overlap space.

3.3 Mutual information and MMSE for angular synchronization

A complete characterization of the information-theoretic limits of inference and the possible existence of computationally-hard SNR regimes may be obtained via an analysis of the global optimization landscape of Ψ_{gs} . To our knowledge, this has been carried out only for the $\mathbb{Z}/2\mathbb{Z}$ -synchronization example, in [DAM16].

In this section, we develop a similar characterization for single-channel angular synchronization over $\mathbb{S}\mathbb{O}(2)$, corresponding to Example 3.4 with $L = 1$ and Example 3.5 with $k = 2$. This is a model with the pairwise observations

$$\mathbf{y}^{(ij)} = \sqrt{\lambda} \mathbf{g}_*^{(i)\top} \mathbf{g}_*^{(j)} + \sqrt{N} \mathbf{z}^{(ij)} = \sqrt{\lambda} \begin{pmatrix} \cos(\theta_j - \theta_i) & -\sin(\theta_j - \theta_i) \\ \sin(\theta_j - \theta_i) & \cos(\theta_j - \theta_i) \end{pmatrix} + \sqrt{N} \mathbf{z}^{(ij)} \quad \text{for } 1 \leq i < j \leq N \quad (38)$$

where $\theta_1, \dots, \theta_N \stackrel{iid}{\sim} \text{Unif}([0, 2\pi))$. Averaging the two measurements of $\cos(\theta_j - \theta_i)$ and $\sin(\theta_j - \theta_i)$ in each observation $\mathbf{y}^{(ij)}$, the model is equivalent to the phase-synchronization model [Bou16] over $\mathbb{U}(1)$ with complex observations

$$y_{ij} = \sqrt{\lambda} e^{i(\theta_j - \theta_i)} + \sqrt{N} z_{ij} \in \mathbb{C}, \quad \Re z^{(ij)}, \Im z^{(ij)} \stackrel{iid}{\sim} \mathcal{N}(0, \frac{1}{2}).$$

Some partial analyses of the replica potential in this model were carried out in [JMRT16, Section 7.2.2], and it was shown in [PWBM16, Theorem 6.11] using an alternative second-moment-method calculation that $\lambda_c = 1$ is the (information-theoretic) threshold for contiguity with the null model $\mathbf{y}^{(ij)} = \sqrt{N} \mathbf{z}^{(ij)}$. Here, we extend these results by showing that the replica potential has a single unique local maximizer $\mathbf{q} \in \text{Sym}_{\geq 0}^{2 \times 2}$,

which is non-zero if and only if $\lambda > 1$, thus providing a full characterization of the Bayes-optimal MMSE and confirming the absence of a statistical-computational gap in this model for any positive λ .

We begin with a general statement that optimization of the replica potential Ψ_{gs} may be restricted to overlaps $\mathbf{q} = (\mathbf{q}_1, \dots, \mathbf{q}_L)$ where each \mathbf{q}_ℓ is a positive multiple of the identity, if \mathcal{G} is abelian and each ϕ_ℓ is real-irreducible. (Each representation must then take values in $\mathbb{R}^{1 \times 1}$ or $\mathbb{R}^{2 \times 2}$, c.f. Corollary D.14, so this statement pertains to the structure of \mathbf{q}_ℓ corresponding to the 2-dimensional representations ϕ_ℓ .)

Proposition 3.9. *Suppose \mathcal{G} is any abelian group, and ϕ_1, \dots, ϕ_L are real-irreducible. If $\mathbf{q} = (\mathbf{q}_\ell)_{\ell=1}^L \in \text{Sym}_{\geq 0}$ is a critical point or local maximizer of Ψ_{gs} , then each \mathbf{q}_ℓ is a scalar multiple of the identity.*

Restricting to scalar multiples of the identity $\mathbf{q} = q I_{2 \times 2}$ with $q \geq 0$, the replica potential takes the form

$$\Psi_{\text{gs}}(q I_{2 \times 2}) = -\frac{\lambda q^2}{2} + \lambda q - i(\lambda q). \quad (39)$$

Here, by (27), $i(\gamma)$ is the mutual information between \mathbf{g}_* and \mathbf{y} in a single-letter model

$$\mathbf{y} = \sqrt{\gamma} \mathbf{g}_* + \mathbf{z} \quad (40)$$

with $\mathbf{g}_* \sim \text{Haar}(\mathbb{S}\mathbb{O}(2))$ and a noise matrix $\mathbf{z} \in \mathbb{R}^{2 \times 2}$ having i.i.d. $\mathcal{N}(0, 1)$ entries. By the i-mmse relation [GSV05], critical points q_* of $\Psi_{\text{gs}}(q I_{2 \times 2})$ correspond to solutions of the fixed-point equation

$$q_* = 1 - \frac{1}{2} \text{mmse}(\lambda q_*) \quad (41)$$

where $\text{mmse}(\gamma) = \mathbb{E} \|\mathbf{g}_* - \mathbb{E}[\mathbf{g} | \mathbf{y}]\|_F^2 = 2 - \mathbb{E} \|\mathbb{E}[\mathbf{g} | \mathbf{y}]\|_F^2$ is the minimum mean-squared-error for estimating \mathbf{g}_* in the single-letter model (40).

The following is our main result for $\mathbb{S}\mathbb{O}(2)$ -synchronization.

Theorem 3.10. *For the $\mathbb{S}\mathbb{O}(2)$ -synchronization model (38), all critical points of $\Psi_{\text{gs}}(\mathbf{q})$ are given by*

$$\{\mathbf{q} \in \text{Sym}_{\geq 0}^{2 \times 2} : \nabla \Psi_{\text{gs}}(\mathbf{q}) = 0\} = \{q_* I_{2 \times 2} : q_* \text{ solves (41)}\}. \quad (42)$$

If $\lambda \leq \lambda_c := 1$, then 0 is the only solution of (41), $\mathbf{q} = \mathbf{0}$ is the unique global maximizer of Ψ_{gs} over $\text{Sym}_{\geq 0}^{2 \times 2}$, and

$$\lim_{n \rightarrow \infty} \frac{1}{N} I(\Theta_*, Y) = \frac{\lambda}{2} \quad \text{and} \quad \lim_{N \rightarrow \infty} \text{MMSE} = 2,$$

and for any $\epsilon > 0$, there exists constants $C, c > 0$ depending only on ϵ such that

$$\mathbb{E} \left\langle \mathbf{1} \left\{ \left\| \frac{1}{N} \sum_{i=1}^N \mathbf{g}^{(i)\top} \mathbf{g}_*^{(i)} \right\|_F^2 > \frac{\epsilon}{\lambda} \right\} \right\rangle \leq C e^{-cN}.$$

If $\lambda > \lambda_c := 1$, then there exists a unique positive solution $q_* > 0$ of (41), $\mathbf{q} = q_* I_{2 \times 2}$ is the unique global maximizer of Ψ_{gs} over $\text{Sym}_{\geq 0}^{2 \times 2}$, and

$$\lim_{N \rightarrow \infty} \frac{1}{N} I(\Theta_*, Y) = \frac{\lambda}{2} - \Psi_{\text{gs}}(q_* I_{2 \times 2}) \quad \text{and} \quad \lim_{N \rightarrow \infty} \text{MMSE} = 2 - 2q_*^2,$$

and for any $\epsilon > 0$, there exists constants $C, c > 0$ depending only on ϵ such that

$$\mathbb{E} \left\langle \mathbf{1} \left\{ \left\| \frac{1}{N} \sum_{i=1}^N \mathbf{g}^{(i)\top} \mathbf{g}_*^{(i)} - q_* \mathbf{h} \right\|_F^2 > \frac{\epsilon}{\lambda} \text{ for all } \mathbf{h} \in \mathbb{S}\mathbb{O}(2) \right\} \right\rangle \leq C e^{-cN}.$$

Remark 3.11. The reduction (42) to diagonal overlap matrices \mathbf{q} is possible because $\mathbb{SO}(2)$ is abelian. The analogous statement in the non-abelian setting of $\mathbb{SO}(k)$ -synchronization for $k \geq 3$ is false: We show in Proposition B.2 that for any $k \geq 3$ and $\lambda > \lambda_c := k$, Ψ_{gs} has a critical point that is not a multiple of the identity. This suggests that analyses of the global optimization landscape of Ψ_{gs} may need to be multivariate in nature, and it remains an open question to fully characterize this landscape for $\mathbb{SO}(k)$ -synchronization when $k \geq 3$ or, more generally, for any non-abelian group \mathcal{G} .

4 Quadratic assignment

We transition to a second application of the general results in Section 2, and study a quadratic assignment model for inference over the symmetric group. Here, the signal and signal prior do not have the “product structure” of group synchronization.

Let \mathcal{X} be a compact space and $\kappa : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ a pairwise similarity kernel, both independent of N . We observe samples $x_1, \dots, x_N \in \mathcal{X}$, together with noisy pairwise similarities of a permutation of these samples,

$$y_{ij} = \kappa(x_{\pi_*(i)}, x_{\pi_*(j)}) + \sqrt{N}z_{ij} \text{ for each } 1 \leq i < j \leq N. \quad (43)$$

Here $z_{ij} \stackrel{iid}{\sim} \mathcal{N}(0, 1)$, and $\pi_* \in \mathbb{S}_N$ is an unknown permutation of interest, assumed to have uniform prior on the symmetric group \mathbb{S}_N of all permutations of N elements.

We will characterize the asymptotic mutual information $I(\pi_*, Y)$ between the latent permutation π_* and observations $Y = (y_{ij})_{i < j}$, under the following assumptions on \mathcal{X} , κ , and x_1, \dots, x_N as $N \rightarrow \infty$.

Assumption 4.1. (a) \mathcal{X} is a compact space, and $\kappa : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a continuous positive-semidefinite kernel, i.e. $\kappa(x_i, x_j)_{i,j=1}^m \in \mathbb{R}^{m \times m}$ is positive-semidefinite for any $m \geq 1$ and $x_1, \dots, x_m \in \mathcal{X}$.

(b) There exists a probability distribution ρ on \mathcal{X} such that, as $N \rightarrow \infty$, the empirical law $\frac{1}{N} \sum_{i=1}^N \delta_{x_i}$ converges weakly to ρ .

Under Assumption 4.1, κ is a Mercer kernel admitting the following approximation by eigenfunctions, see e.g. [Wai19, Theorem 12.20].

Theorem 4.2 (Mercer’s theorem). *Suppose Assumption 4.1 holds. Then there exists an orthonormal basis of eigenfunctions $\{f_\ell\}_{\ell=1}^\infty$ of $L^2(\mathcal{X}, \rho)$ and eigenvalues $\mu_1 \geq \mu_2 \geq \mu_3 \geq \dots \geq 0$ such that $\int_{\mathcal{X}} \kappa(x, y) f_\ell(y) \rho(dy) = \mu_\ell f_\ell(x)$. Furthermore, κ admits the expansion*

$$\kappa(x, y) = \sum_{\ell=1}^{\infty} \mu_\ell f_\ell(x) f_\ell(y)$$

where this series converges absolutely and uniformly over all $x, y \in \mathcal{X}$.

We define from this eigenfunction expansion, for each $L \geq 1$, the truncated kernel

$$\kappa^L(x, y) := \sum_{\ell=1}^L \mu_\ell f_\ell(x) f_\ell(y). \quad (44)$$

The model defined by κ^L in place of κ falls into the framework of Section 2, where $\mathcal{G}_N \equiv \mathbb{S}_N$ is the symmetric group, and the feature map $\phi : \mathbb{S}_N \rightarrow \mathcal{H}^N$ has components

$$\phi(\pi)_i = (\sqrt{\mu_1} f_1(x_{\pi(i)}), \dots, \sqrt{\mu_L} f_L(x_{\pi(i)})) \in \mathcal{H} \equiv \mathbb{R}^L. \quad (45)$$

The bilinear maps $\bullet : \mathcal{H} \times \mathcal{H} \rightarrow \mathcal{K} \equiv \mathbb{R}$ and $\otimes : \mathcal{H} \times \mathcal{H} \rightarrow \mathcal{L} \equiv \mathbb{R}^{L \times L}$ and the inclusion map $\iota : \mathcal{L} \rightarrow B(\mathcal{H})$ are given by

$$\mathbf{a} \bullet \mathbf{b} = \mathbf{a}^\top \mathbf{b}, \quad \mathbf{a} \otimes \mathbf{b} = \mathbf{a} \mathbf{b}^\top, \quad \iota(\mathbf{q})\mathbf{a} = \mathbf{q}\mathbf{a}, \quad (46)$$

where we equip $\mathcal{H}, \mathcal{K}, \mathcal{L}$ with their usual Euclidean inner-products. Our analyses will first characterize the asymptotic mutual information between π_* and observations $Y^L = \{y_{ij}^L\}_{i < j}$ defined with the truncated kernel κ^L , and then take a limit $L \rightarrow \infty$ to describe the mutual information for the original observations Y .

Asymptotic mutual information. Fixing any $L \geq 1$ and an overlap matrix $\mathbf{q} \in \text{Sym}_{\geq 0}^{L \times L}$, denote $\mathbf{u}(x) = (\sqrt{\mu_1}f_1(x), \dots, \sqrt{\mu_L}f_L(x)) \in \mathbb{R}^L$ and consider a linear observation model

$$\mathbf{y}_i = \mathbf{q}^{1/2} \mathbf{u}(x_{\pi_*(i)}) + \mathbf{z}_i \in \mathbb{R}^L \text{ for } i = 1, \dots, N \quad (47)$$

where $\pi_* \sim \text{Haar}(\mathbb{S}_N)$ and $\{\mathbf{z}_i\}_{i=1}^N \stackrel{iid}{\sim} \mathcal{N}(0, I_{L \times L})$. Consider also the single-letter model

$$\mathbf{y} = \mathbf{q}^{1/2} \mathbf{u}(x) + \mathbf{z} \in \mathbb{R}^L \quad (48)$$

where $x \sim \rho$ is a single random sample in \mathcal{X} , and $\mathbf{z} \sim \mathcal{N}(0, I)$. It is direct to check, as in (16), that the mutual information in the model (48) is given by $i(x, \mathbf{y}) = -\frac{1}{4} \|\mathbf{q}\|_F^2 + \frac{1}{2} \mathbb{E}_{x_*} \text{Tr} \mathbf{u}(x_*)^\top \mathbf{q} \mathbf{u}(x_*) - \Psi_{\text{qa}}^L(\mathbf{q})$, for the potential function

$$\Psi_{\text{qa}}^L(\mathbf{q}) = -\frac{1}{4} \|\mathbf{q}\|_F^2 + \mathbb{E}_{x_*, \mathbf{z}} \log \mathbb{E}_x \exp \left(-\frac{1}{2} \mathbf{u}(x)^\top \mathbf{q} \mathbf{u}(x) + \mathbf{u}(x)^\top \mathbf{q} \mathbf{u}(x_*) + \mathbf{u}(x)^\top \mathbf{q}^{1/2} \mathbf{z} \right). \quad (49)$$

Here, \mathbb{E}_x is over $x \sim \rho$ in \mathcal{X} , and $\mathbb{E}_{x_*, \mathbf{z}}$ is over independent $x_* \sim \rho$ and $\mathbf{z} \sim \mathcal{N}(0, I)$.

Inference in the model (47) may be understood as the task of estimating $\boldsymbol{\theta}_i = \mathbf{q}^{1/2} \mathbf{u}(x_{\pi_*(i)}) \in \mathbb{R}^L$ for $i = 1, \dots, N$ from observations $\mathbf{y}_i = \boldsymbol{\theta}_i + \mathbf{z}_i$, given only the empirical distribution of the values $\{\boldsymbol{\theta}_i\}_{i=1}^N$ but not their ordering. In contrast, inference in the model (48) is the task of estimating $\boldsymbol{\theta}_i$ from an observation $\mathbf{y}_i = \boldsymbol{\theta}_i + \mathbf{z}_i$ assuming a Bayesian prior for $\boldsymbol{\theta}_i$. Comparisons between these two tasks underlie the classical literature on empirical Bayes estimation in compound decision problems; in particular, the efficiency of coordinate-separable decision rules within the class of all decision rules for the former model (47) has been investigated in [HR55, GR09].

Leveraging the main result of [GR09], the following lemma first shows that the signal-observation mutual information in the linear observation model (47) coincides, to leading asymptotic order, with that in the scalar model (48).

Lemma 4.3. *Suppose Assumption 4.1 holds, and fix any $L \geq 1$ and $\mathbf{q} \in \text{Sym}_{\geq 0}^{L \times L}$. Let $i(\pi_*, Y_{\text{lin}})$ be the mutual information between $\pi_* \in \mathbb{S}_N$ and $Y_{\text{lin}} = \{\mathbf{y}_i\}_{i=1}^N$ in the model (47). Then*

$$\lim_{N \rightarrow \infty} \frac{1}{N} i(\pi_*, Y_{\text{lin}}) = i(x, \mathbf{y}) := -\frac{1}{4} \|\mathbf{q}\|_F^2 + \frac{1}{2} \mathbb{E}_{x_*} \text{Tr} \mathbf{u}(x_*)^\top \mathbf{q} \mathbf{u}(x_*) - \Psi_{\text{qa}}^L(\mathbf{q}).$$

The general framework of Section 2 then allows us to relate $i(\pi_*, Y_{\text{lin}})$ with the mutual information $I(\pi_*, Y)$ in the quadratic assignment model (43), yielding the following main result of this section.

Theorem 4.4. *Suppose Assumption 4.1 holds. Then there exists a finite limit*

$$\Psi_\infty = \lim_{L \rightarrow \infty} \sup_{\mathbf{q} \in \text{Sym}_{\geq 0}^{L \times L}} \Psi_{\text{qa}}^L(\mathbf{q}),$$

and the mutual information $I(\pi_*, Y)$ between $\pi_* \sim \mathbb{S}_N$ and $Y = \{y_{ij}\}_{i < j}$ in the model (43) satisfies

$$\lim_{N \rightarrow \infty} \frac{1}{N} I(\pi_*, Y) = \frac{1}{4} \mathbb{E}_{x, x' \stackrel{iid}{\sim} \rho} [\kappa(x, x')^2] - \Psi_\infty. \quad (50)$$

The limit value in (50) may be understood as the mutual information between a signal vector (x_{*1}, \dots, x_{*N}) having i.i.d. prior $x_{*i} \stackrel{iid}{\sim} \rho$, and observations

$$y_{ij} = \kappa(x_{*i}, x_{*j}) + \sqrt{N} z_{ij} \text{ for } 1 \leq i < j \leq N.$$

In the setting where κ has a finite expansion into eigenfunctions, i.e. $\kappa^L = \kappa$ for some finite L , this is the mutual information in a usual low-rank matrix estimation model with i.i.d. signal prior. Informally, Theorem 4.4 shows that in a bounded SNR regime of the model (43) where the kernel eigenvalues μ_1, μ_2, \dots are fixed independently of N , observing the exact sample points x_1, \dots, x_N is asymptotically no more informative for estimating $\kappa(x_{\pi_*(i)}, x_{\pi_*(j)})_{i < j}$ than knowing the ‘‘prior distribution’’ ρ corresponding to the limit of their empirical law.

5 Conclusion

In this work, we have studied the two models of group synchronization and quadratic assignment on pairs of noisy positive-semidefinite kernel matrices observed with Gaussian noise. These problems share a common structure of estimating a latent element G_* of a high-dimensional group from pairwise observations. Assuming a Bayesian setting with Haar-uniform prior for G_* , we have derived under a common framework the limit of the signal-observation mutual information in both models, in an asymptotic regime of bounded SNR. For group synchronization, we have given a complete characterization of the algorithmic phase transition threshold for $\mathbf{q} = \mathbf{0}$ to locally optimize the replica potential in general groups. For quadratic assignment, we have shown that the signal-observation mutual information is asymptotically equivalent to that in a low-rank matrix estimation model with i.i.d. signal prior.

The framework developed here is fairly general, and may apply to other Bayesian inference problems of this form, where the underlying group \mathcal{G}_N does not necessarily have a product structure. We have analyzed two examples in which the linear observation model (to which the original quadratic model is compared) admits a reasonably simple direct analysis. In applications with other group structures, as well as in other regimes of SNR, the linear model itself may exhibit other types of asymptotic behaviors, and we believe this may be interesting to investigate in future work.

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A Proofs for the general model

Throughout this section, we write as shorthand

$$\phi = \phi(G), \quad \phi' = \phi(G'), \quad \phi_* = \phi(G_*)$$

and abbreviate $\mathcal{F} \equiv \mathcal{F}_N$, $\Psi \equiv \Psi_N$. Define the Hamiltonian

$$\begin{aligned} \tilde{H}(G; G_*, Z) = & \sum_{1 \leq i < j \leq N} -\frac{1}{2N} \|\phi_i \bullet \phi_j\|_{\mathcal{K}}^2 + \frac{1}{N} \langle \phi_i \bullet \phi_j, \phi_{*i} \bullet \phi_{*j} \rangle_{\mathcal{K}} + \frac{1}{\sqrt{N}} \langle \phi_i \bullet \phi_j, \mathbf{z}_{ij} \rangle_{\mathcal{K}} \\ & + \sum_{i=1}^N -\frac{1}{4N} \|\phi_i \bullet \phi_i\|_{\mathcal{K}}^2 + \frac{1}{2N} \langle \phi_i \bullet \phi_i, \phi_{*i} \bullet \phi_{*i} \rangle_{\mathcal{K}} + \frac{1}{\sqrt{2N}} \langle \phi_i \bullet \phi_i, \mathbf{z}_{ii} \rangle_{\mathcal{K}} \end{aligned} \quad (51)$$

where $\{\mathbf{z}_{ii}\}_{i=1}^N$ are additional standard Gaussian noise vectors in \mathcal{K} , independent of G_* and of $\{\mathbf{z}_{ij}\}_{i < j}$. Then $\exp \tilde{H}(G; G_*, Z)$ is proportional to the posterior density of G in the model (2) with additional observations

$$\mathbf{y}_{ii} = \phi_i \bullet \phi_i + \sqrt{2N} \mathbf{z}_{ii} \quad \text{for } i = 1, \dots, N.$$

We will establish lower and upper bounds for the perturbed free energy

$$\tilde{\mathcal{F}} = \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp \tilde{H}(G; G_*, Z)$$

and remove this perturbation at the conclusion of the proof.

A.1 Free energy lower bound

We first prove the following lower bound for $\tilde{\mathcal{F}}$.

Lemma A.1. *Under Assumption 2.1,*

$$\tilde{\mathcal{F}} \geq \sup_{\mathbf{q} \in \mathcal{Q}} \Psi(\mathbf{q}).$$

Fixing any $\mathbf{q} \in \mathcal{Q}$, for every $0 \leq t \leq 1$, consider the observations

$$\begin{cases} \mathbf{y}_{ij}^{(t)} = \sqrt{t} \phi_{*i} \bullet \phi_{*j} + \sqrt{N} \mathbf{z}_{ij} & \text{for all } 1 \leq i < j \leq N \\ \mathbf{y}_{ii}^{(t)} = \sqrt{t} \phi_{*i} \bullet \phi_{*i} + \sqrt{2N} \mathbf{z}_{ii} & \text{for all } i = 1, \dots, N \\ \mathbf{y}_i^{(t)} = \sqrt{(1-t)} \mathbf{q}^{1/2} \phi_{*i} + \mathbf{z}_i & \text{for all } i = 1, \dots, N \end{cases} \quad (52)$$

where $\{\mathbf{z}_{ij}\}_{i < j}$ and $\{\mathbf{z}_i\}_{i=1}^N$ are standard Gaussian noise vectors in \mathcal{K} and \mathcal{H} respectively, independent of each other and of $G_* \sim \text{Haar}(\mathcal{G}_N)$. The posterior distribution of G given the joint observations (52) is proportional to $\exp \tilde{H}_t(G; G_*, Z)$ for the interpolating Hamiltonian

$$\begin{aligned} \tilde{H}_t(G; G_*, Z) = & \sum_{1 \leq i < j \leq N} -\frac{t}{2N} \|\phi_i \bullet \phi_j\|_{\mathcal{K}}^2 + \frac{t}{N} \langle \phi_i \bullet \phi_j, \phi_{*i} \bullet \phi_{*j} \rangle_{\mathcal{K}} + \sqrt{\frac{t}{N}} \langle \phi_i \bullet \phi_j, \mathbf{z}_{ij} \rangle_{\mathcal{K}} \\ & + \sum_{i=1}^N -\frac{t}{4N} \|\phi_i \bullet \phi_i\|_{\mathcal{K}}^2 + \frac{t}{2N} \langle \phi_i \bullet \phi_i, \phi_{*i} \bullet \phi_{*i} \rangle_{\mathcal{K}} + \sqrt{\frac{t}{2N}} \langle \phi_i \bullet \phi_i, \mathbf{z}_{ii} \rangle_{\mathcal{K}} \\ & + \sum_{i=1}^N -\frac{(1-t)}{2} \|\mathbf{q}^{1/2} \phi_i\|_{\mathcal{H}}^2 + (1-t) \langle \mathbf{q}^{1/2} \phi_i, \mathbf{q}^{1/2} \phi_{*i} \rangle_{\mathcal{H}} + \sqrt{1-t} \langle \mathbf{q}^{1/2} \phi_i, \mathbf{z}_i \rangle_{\mathcal{H}}. \end{aligned} \quad (53)$$

For $0 \leq t \leq 1$, we denote the posterior mean $\langle f(G) \rangle_t = \frac{\mathbb{E}_G[f(G) \exp \tilde{H}_t(G; G_*, Z)]}{\mathbb{E}_G[\exp \tilde{H}_t(G; G_*, Z)]}$ (not to be confused with the inner-product notations $\langle \cdot, \cdot \rangle_{\mathcal{K}}$ and $\langle \cdot, \cdot \rangle_{\mathcal{H}}$). The Nishimori identity holds for $\mathbb{E} \langle \cdot \rangle_t$ by Bayes' rule in the model (52). Define the interpolating free energy

$$\tilde{\mathcal{F}}(t) = \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp \tilde{H}_t(G; G_*, Z)$$

where $\tilde{\mathcal{F}}(1) = \tilde{\mathcal{F}}$ is the free energy of interest. At $t = 0$, applying the identity

$$\sum_{i=1}^N \langle \mathbf{q}^{1/2} \phi_i, \mathbf{q}^{1/2} \phi'_i \rangle_{\mathcal{H}} = \sum_{i=1}^N \langle \phi_i, \mathbf{q} \phi'_i \rangle_{\mathcal{H}} = \sum_{i=1}^N \langle \mathbf{q}, \phi_i \otimes \phi'_i \rangle_{\mathcal{L}} = N \langle \mathbf{q}, Q(G, G') \rangle_{\mathcal{L}} \quad (54)$$

for any $G, G' \in \mathcal{G}_N$, and the group symmetry $Q(G, G) = Q(\text{Id}, \text{Id})$, we have

$$\begin{aligned} \tilde{\mathcal{F}}(0) &= -\frac{1}{2} \langle \mathbf{q}, Q(\text{Id}, \text{Id}) \rangle_{\mathcal{L}} + \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp \left(N \langle \mathbf{q}, Q(G, G_*) \rangle_{\mathcal{L}} + \sum_{i=1}^N \langle \mathbf{q}^{1/2} \phi_i, \mathbf{z}_i \rangle_{\mathcal{H}} \right) \\ &= \Psi(\mathbf{q}) + \frac{1}{4} \|\mathbf{q}\|_{\mathcal{L}}^2 \end{aligned} \quad (55)$$

A calculation based on Gaussian integration by parts shows the derivative of $\tilde{\mathcal{F}}(t)$.

Proposition A.2.

$$\tilde{\mathcal{F}}'(t) = -\frac{1}{4} \|\mathbf{q}\|_{\mathcal{L}}^2 + \frac{1}{4} \mathbb{E}_{G_*, Z} \langle \|Q(G, G_*) - \mathbf{q}\|_{\mathcal{L}}^2 \rangle_t.$$

Proof. First note that

$$\tilde{\mathcal{F}}'(t) = \frac{1}{N} \mathbb{E}_{G_*, Z} \left\langle \frac{d}{dt} \tilde{H}_t(G; G_*, Z) \right\rangle_t$$

where we have

$$\begin{aligned} \frac{d}{dt} \tilde{H}_t(G; G_*, Z) &= \sum_{i < j} -\frac{1}{2N} \|\phi_i \bullet \phi_j\|_{\mathcal{K}}^2 + \frac{1}{N} \langle \phi_i \bullet \phi_j, \phi_{*i} \bullet \phi_{*j} \rangle_{\mathcal{K}} + \frac{1}{2\sqrt{tN}} \langle \phi_i \bullet \phi_j, \mathbf{z}_{ij} \rangle_{\mathcal{K}} \\ &\quad + \sum_{i=1}^N -\frac{1}{4N} \|\phi_i \bullet \phi_i\|_{\mathcal{K}}^2 + \frac{1}{2N} \langle \phi_i \bullet \phi_i, \phi_{*i} \bullet \phi_{*i} \rangle_{\mathcal{K}} + \frac{1}{2\sqrt{2tN}} \langle \phi_i \bullet \phi_i, \mathbf{z}_{ii} \rangle_{\mathcal{K}} \\ &\quad + \sum_{i=1}^N \frac{1}{2} \|\mathbf{q}^{1/2} \phi_i\|_{\mathcal{H}}^2 - \langle \mathbf{q}^{1/2} \phi_i, \mathbf{q}^{1/2} \phi_{*i} \rangle_{\mathcal{H}} - \frac{1}{2\sqrt{1-t}} \langle \mathbf{q}^{1/2} \phi_i, \mathbf{z}_i \rangle_{\mathcal{H}}. \end{aligned}$$

Applying Gaussian integration by parts and denoting $\phi'_i = \phi(G')_i$ for an independent sample G' from the posterior law,

$$\begin{aligned} \mathbb{E}_Z \left\langle \frac{1}{2\sqrt{tN}} \langle \phi_i \bullet \phi_j, \mathbf{z}_{ij} \rangle_{\mathcal{K}} \right\rangle_t &= \frac{1}{2N} \mathbb{E}_{G_*, Z} \left\langle \|\phi_i \bullet \phi_j\|_{\mathcal{K}}^2 - \langle \phi_i \bullet \phi_j, \phi'_i \bullet \phi'_j \rangle_{\mathcal{K}} \right\rangle_t, \\ \mathbb{E}_Z \left\langle \frac{1}{2\sqrt{2tN}} \langle \phi_i \bullet \phi_i, \mathbf{z}_{ii} \rangle_{\mathcal{K}} \right\rangle_t &= \frac{1}{4N} \mathbb{E}_{G_*, Z} \left\langle \|\phi_i \bullet \phi_i\|_{\mathcal{K}}^2 - \langle \phi_i \bullet \phi_i, \phi'_i \bullet \phi'_i \rangle_{\mathcal{K}} \right\rangle_t, \\ \mathbb{E}_Z \left\langle \frac{1}{2\sqrt{1-t}} \langle \mathbf{q}^{1/2} \phi_i, \mathbf{z}_i \rangle_{\mathcal{H}} \right\rangle_t &= \frac{1}{2} \mathbb{E}_{G_*, Z} \left\langle \|\mathbf{q}^{1/2} \phi_i\|_{\mathcal{H}}^2 - \langle \mathbf{q}^{1/2} \phi_i, \mathbf{q}^{1/2} \phi'_i \rangle_{\mathcal{H}} \right\rangle_t. \end{aligned}$$

Hence

$$\begin{aligned}
\tilde{\mathcal{F}}'(t) &= \frac{1}{N} \mathbb{E}_{G_*, Z} \left\langle \frac{1}{N} \sum_{i < j} \langle \phi_i \bullet \phi_j, \phi_{*i} \bullet \phi_{*j} \rangle_{\mathcal{K}} - \frac{1}{2N} \sum_{i < j} \langle \phi_i \bullet \phi_j, \phi'_i \bullet \phi'_j \rangle_{\mathcal{K}} + \frac{1}{2N} \sum_{i=1}^N \langle \phi_i \bullet \phi_i, \phi_{*i} \bullet \phi_{*i} \rangle_{\mathcal{K}} \right. \\
&\quad \left. - \frac{1}{4N} \sum_{i=1}^N \langle \phi_i \bullet \phi_i, \phi'_i \bullet \phi'_i \rangle_{\mathcal{K}} - \sum_{i=1}^N \langle \mathbf{q}^{1/2} \phi_i, \mathbf{q}^{1/2} \phi_{*i} \rangle_{\mathcal{H}} + \frac{1}{2} \sum_{i=1}^N \langle \mathbf{q}^{1/2} \phi_i, \mathbf{q}^{1/2} \phi'_i \rangle_{\mathcal{H}} \right\rangle_t \\
&= \mathbb{E}_{G_*, Z} \left\langle \frac{1}{2N^2} \sum_{i, j=1}^N \langle \phi_i \bullet \phi_j, \phi_{*i} \bullet \phi_{*j} \rangle_{\mathcal{K}} - \frac{1}{4N^2} \sum_{i, j=1}^N \langle \phi_i \bullet \phi_j, \phi'_i \bullet \phi'_j \rangle_{\mathcal{K}} \right. \\
&\quad \left. - \frac{1}{N} \sum_{i=1}^N \langle \mathbf{q}^{1/2} \phi_i, \mathbf{q}^{1/2} \phi_{*i} \rangle_{\mathcal{H}} + \frac{1}{2N} \sum_{i=1}^N \langle \mathbf{q}^{1/2} \phi_i, \mathbf{q}^{1/2} \phi'_i \rangle_{\mathcal{H}} \right\rangle_t.
\end{aligned}$$

By Assumption 2.1, for any $G, G' \in \mathcal{G}_N$, we have

$$\sum_{i, j=1}^N \langle \phi_i \bullet \phi_j, \phi'_i \bullet \phi'_j \rangle_{\mathcal{K}} = \sum_{i, j=1}^N \langle \phi_i \otimes \phi'_i, \phi_j \otimes \phi'_j \rangle_{\mathcal{L}} = N^2 \|Q(G, G')\|_{\mathcal{L}}^2. \quad (56)$$

Applying (54) and (56) to the above gives

$$\tilde{\mathcal{F}}'(t) = \mathbb{E}_{G_*, Z} \left\langle \frac{1}{2} \|Q(G, G_*)\|_{\mathcal{L}}^2 - \frac{1}{4} \|Q(G, G')\|_{\mathcal{L}}^2 - \langle \mathbf{q}, Q(G, G_*) \rangle_{\mathcal{L}} + \frac{1}{2} \langle \mathbf{q}, Q(G, G') \rangle_{\mathcal{L}} \right\rangle_t. \quad (57)$$

Finally, by Nishimori's identity, $\mathbb{E}_{G_*, Z} \langle f(G, G') \rangle_t = \mathbb{E}_{G_*, Z} \langle f(G, G_*) \rangle_t$, so

$$\tilde{\mathcal{F}}'(t) = \mathbb{E}_{G_*, Z} \left\langle \frac{1}{4} \|Q(G, G_*)\|_{\mathcal{L}}^2 - \frac{1}{2} \langle \mathbf{q}, Q(G, G_*) \rangle_{\mathcal{L}} \right\rangle_t = -\frac{1}{4} \|\mathbf{q}\|_{\mathcal{L}}^2 + \frac{1}{4} \mathbb{E}_{G_*, Z} \langle \|Q(G, G_*) - \mathbf{q}\|_{\mathcal{L}}^2 \rangle_t.$$

□

Proof of Lemma A.1. For any $\mathbf{q} \in \mathcal{Q}$, applying (55) and Proposition A.2 with $\|Q(G, G_*) - \mathbf{q}\|_{\mathcal{L}}^2 \geq 0$, we have $\tilde{\mathcal{F}} = \tilde{\mathcal{F}}(0) + \int_0^1 \tilde{\mathcal{F}}'(t) dt \geq \Psi(\mathbf{q})$, and the result follows upon taking a supremum over $\mathbf{q} \in \mathcal{Q}$. □

A.2 Free energy upper bound via the Franz-Parisi potential

In this section, we now prove the following upper bound for $\tilde{\mathcal{F}}$.

Lemma A.3. *In the setting of Theorem 2.2, for any $\epsilon > 0$,*

$$\tilde{\mathcal{F}} \leq \sup_{\mathbf{q} \in \mathcal{Q}} \Psi(\mathbf{q}) + D(\mathcal{G}_N) \sqrt{\frac{L(\epsilon^{1/2}; \mathcal{G}_N)}{N}} + \frac{L(\epsilon^{1/2}; \mathcal{G}_N)}{N} + \frac{\epsilon}{2}. \quad (58)$$

Recall that $Q(G, G_*) = N^{-1} \sum_{i=1}^N \phi(G)_i \otimes \phi(G_*)_i \in \mathcal{L}$. For any $\mathbf{m} \in \mathcal{L}$ and $\epsilon > 0$, define the Franz-Parisi potential

$$\tilde{\Phi}_\epsilon(\mathbf{m}) = \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \left[\mathbf{1}_{\{\|Q(G, G_*) - \mathbf{m}\|_{\mathcal{L}}^2 \leq \epsilon\}} \exp \tilde{H}(G; G_*, Z) \right]. \quad (59)$$

This is the restriction of the free energy to samples G for which $Q(G, G_*)$ falls close to \mathbf{m} . It is clear that $\tilde{\mathcal{F}} \geq \tilde{\Phi}_\epsilon(\mathbf{m})$ for all $\mathbf{m} \in \mathcal{L}$; the following lemma provides a complementary upper bound.

Lemma A.4. *In the setting of Theorem 2.2, for any $\epsilon > 0$,*

$$\tilde{\mathcal{F}} \leq \sup_{\mathbf{m} \in \mathcal{L}} \tilde{\Phi}_\epsilon(\mathbf{m}) + D(\mathcal{G}_N) \sqrt{\frac{L(\epsilon^{1/2}; \mathcal{G}_N)}{N}} + \frac{L(\epsilon^{1/2}; \mathcal{G}_N)}{N}. \quad (60)$$

Proof. Let \mathcal{M} be a $\sqrt{\epsilon}$ -cover of $\text{image}(Q)$ in the norm $\|\cdot\|_{\mathcal{L}}$ with cardinality $\log |\mathcal{M}| = L(\epsilon^{1/2}; \mathcal{G}_N)$. Then for any $G, G_* \in \mathcal{G}_N$, some point of \mathcal{M} must be within $\sqrt{\epsilon}$ -distance of $Q(G, G_*) \in \mathcal{L}$, so we have

$$\begin{aligned} \tilde{\mathcal{F}} &\leq \frac{1}{N} \mathbb{E}_{G_*, Z} \log \sum_{\mathbf{m} \in \mathcal{M}} \mathbb{E}_G \left[\mathbf{1}\{\|Q(G, G_*) - \mathbf{m}\|_{\mathcal{L}}^2 \leq \epsilon\} \exp \tilde{H}(G; G_*, Z) \right] \\ &\leq \mathbb{E}_{G_*, Z} \max_{\mathbf{m} \in \mathcal{M}} \underbrace{\frac{1}{N} \log \mathbb{E}_G \left[\mathbf{1}\{\|Q(G, G_*) - \mathbf{m}\|_{\mathcal{L}}^2 \leq \epsilon\} \exp \tilde{H}(G; G_*, Z) \right]}_{:= \tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m})} + \frac{\log |\mathcal{M}|}{N}. \end{aligned} \quad (61)$$

We apply concentration over $Z = \{\mathbf{z}_{ij}\}_{i \leq j}$ to pass \mathbb{E}_Z inside $\max_{\mathbf{m} \in \mathcal{M}}$. Define $\tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m})$ as in (61), and denote the corresponding Gibbs average $\langle f(G) \rangle = \frac{\mathbb{E}_G[f(G) \mathbf{1}\{\|Q(G, G_*) - \mathbf{m}\|_{\mathcal{L}}^2 \leq \epsilon\} \exp \tilde{H}(G; G_*, Z)]}{\mathbb{E}_G[\mathbf{1}\{\|Q(G, G_*) - \mathbf{m}\|_{\mathcal{L}}^2 \leq \epsilon\} \exp \tilde{H}(G; G_*, Z)]}$ (again not to be confused with the inner-products $\langle \cdot, \cdot \rangle_{\mathcal{K}}$ and $\langle \cdot, \cdot \rangle_{\mathcal{L}}$). Then, differentiating (51) and applying (56) and Jensen's inequality,

$$\begin{aligned} &\sum_{i < j} \|\nabla_{\mathbf{z}_{ij}} \tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m})\|_{\mathcal{K}}^2 + \sum_{i=1}^N \|\nabla_{\mathbf{z}_{ii}} \tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m})\|_{\mathcal{K}}^2 \\ &= \sum_{i < j} \left\| \frac{1}{N} \langle \nabla_{\mathbf{z}_{ij}} \tilde{H}(G; G_*, Z) \rangle \right\|_{\mathcal{K}}^2 + \sum_{i=1}^N \left\| \frac{1}{N} \langle \nabla_{\mathbf{z}_{ii}} \tilde{H}(G; G_*, Z) \rangle \right\|_{\mathcal{K}}^2 \\ &= \frac{1}{2N^3} \sum_{i, j=1}^N \|\langle \phi_i \bullet \phi_j \rangle\|_{\mathcal{K}}^2 \leq \frac{1}{2N^3} \left\langle \sum_{i, j=1}^N \|\phi_i \bullet \phi_j\|_{\mathcal{K}}^2 \right\rangle = \frac{1}{2N} \langle \|Q(G, G)\|_{\mathcal{L}}^2 \rangle \leq \frac{D(\mathcal{G}_N)^2}{2N}. \end{aligned} \quad (62)$$

Therefore, $\tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m})$ is $D(\mathcal{G}_N)/\sqrt{2N}$ -Lipschitz, so $\mathbb{E}_Z e^{\lambda(\tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m}) - \mathbb{E}_Z \tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m}))} \leq e^{\lambda^2 D(\mathcal{G}_N)^2 / 4N}$ for any $\lambda > 0$ by Gaussian concentration of measure [BLB03, Theorem 5.5]. Thus, applying also Jensen's inequality,

$$\begin{aligned} \mathbb{E}_Z \max_{\mathbf{m} \in \mathcal{M}} \left(\tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m}) - \mathbb{E}_Z \tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m}) \right) &\leq \mathbb{E}_Z \frac{1}{\lambda} \log \sum_{\mathbf{m} \in \mathcal{M}} e^{\lambda(\tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m}) - \mathbb{E}_Z \tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m}))} \\ &\leq \frac{1}{\lambda} \log \sum_{\mathbf{m} \in \mathcal{M}} \mathbb{E}_Z e^{\lambda(\tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m}) - \mathbb{E}_Z \tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m}))} \leq \frac{1}{\lambda} \log |\mathcal{M}| + \frac{\lambda D(\mathcal{G}_N)^2}{4N}. \end{aligned}$$

Optimizing over λ and applying this to (61), we get

$$\tilde{\mathcal{F}} \leq \mathbb{E}_{G_*} \max_{\mathbf{m} \in \mathcal{M}} \mathbb{E}_Z \tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m}) + D(\mathcal{G}_N) \sqrt{\frac{\log |\mathcal{M}|}{N}} + \frac{\log |\mathcal{M}|}{N}. \quad (63)$$

Next, we claim by the group symmetry $Q(G, G_*) = Q(G_*^{-1}G, \text{Id})$ that $\mathbb{E}_Z \tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m})$ has the same value for all $G_* \in \mathcal{G}_N$, and hence equals $\tilde{\Phi}_\epsilon(\mathbf{m})$. Indeed, denoting

$$Z(G) = \sum_{i < j} \frac{1}{\sqrt{N}} \langle \phi_i \bullet \phi_j, \mathbf{z}_{ij} \rangle_{\mathcal{K}} + \sum_{i=1}^N \frac{1}{\sqrt{2N}} \langle \phi_i \bullet \phi_i, \mathbf{z}_{ii} \rangle_{\mathcal{K}}$$

and applying the definition of $\tilde{H}(G; G_*, Z)$ from (51) and the identity (56), we have

$$\tilde{H}(G; G_*, Z) = -\frac{N}{4} Q(G, G) + \frac{N}{2} Q(G, G_*) + Z(G) = -\frac{N}{4} Q(\text{Id}, \text{Id}) + \frac{N}{2} Q(G_*^{-1}G, \text{Id}) + Z(G).$$

Here, $\{Z(G)\}_{G \in \mathcal{G}_N}$ is a mean-zero Gaussian process with covariance

$$\mathbb{E}[Z(G)Z(G')] = \sum_{i < j} \frac{1}{N} \langle \phi_i \bullet \phi_j, \phi'_i \bullet \phi'_j \rangle_{\mathcal{K}} + \sum_{i=1}^N \frac{1}{2N} \langle \phi_i \bullet \phi_i, \phi'_i \bullet \phi'_i \rangle_{\mathcal{K}} = \frac{N}{2} Q(G, G').$$

For any fixed $G_* \in \mathcal{G}_N$, the process $\{Z(G)\}_{G \in \mathcal{G}_N}$ is then equal in law to $\{Z(G_*^{-1}G)\}_{G \in \mathcal{G}_N}$, because the latter process is also mean-zero with the same covariance

$$\mathbb{E}[Z(G_*^{-1}G)Z(G_*^{-1}G')] = \frac{N}{2} Q(G_*^{-1}G, G_*^{-1}G') = \frac{N}{2} Q(G, G').$$

Then, applying also the invariance of Haar measure, this implies

$$\begin{aligned} & \mathbb{E}_Z \tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m}) \\ &= \frac{1}{N} \mathbb{E}_Z \log \mathbb{E}_G \left[\mathbf{1}\{\|Q(G_*^{-1}G, \text{Id}) - \mathbf{m}\|_{\mathcal{L}}^2 \leq \epsilon\} \exp\left(-\frac{N}{4} Q(\text{Id}, \text{Id}) + \frac{N}{2} Q(G_*^{-1}G, \text{Id}) + Z(G_*^{-1}G)\right) \right] \\ &= \frac{1}{N} \mathbb{E}_Z \log \mathbb{E}_G \left[\mathbf{1}\{\|Q(G, \text{Id}) - \mathbf{m}\|_{\mathcal{L}}^2 \leq \epsilon\} \exp\left(-\frac{N}{4} Q(\text{Id}, \text{Id}) + \frac{N}{2} Q(G, \text{Id}) + Z(G)\right) \right] = \mathbb{E}_Z \tilde{\Phi}_\epsilon(\text{Id}, Z; \mathbf{m}) \end{aligned} \quad (64)$$

so $\mathbb{E}_Z \tilde{\Phi}_\epsilon(G_*, Z; \mathbf{m}) = \tilde{\Phi}_\epsilon(\mathbf{m})$ for all $G_* \in \mathcal{G}_N$, as claimed. Then (63) is equal to the desired upper bound for $\tilde{\mathcal{F}}$, completing the proof. \square

Next, we apply an interpolation argument to upper bound the Franz-Parisi potential (59). For any $\mathbf{m} \in \mathcal{L}$ and $\mathbf{q} \in \mathcal{Q} \subset \mathcal{L}$, define

$$\begin{aligned} \Psi(\mathbf{q}, \mathbf{m}) &= \frac{1}{4} \|\mathbf{q}\|_{\mathcal{L}}^2 - \frac{1}{2} \|\mathbf{m}\|_{\mathcal{L}}^2 - \frac{1}{2} \langle \mathbf{q}, Q(\text{Id}, \text{Id}) \rangle_{\mathcal{L}} \\ &\quad + \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp\left(N \langle \mathbf{m}, Q(G, G_*) \rangle_{\mathcal{L}} + \sum_{i=1}^N \langle \mathbf{q}^{1/2} \phi(G)_i, \mathbf{z}_i \rangle_{\mathcal{H}}\right) \end{aligned}$$

Note that $\Psi(\mathbf{q}, \mathbf{q}) = \Psi(\mathbf{q})$ as defined in (14).

Lemma A.5. *For any $\mathbf{m} \in \mathcal{L}$, $\mathbf{q} \in \mathcal{Q}$, and $\epsilon > 0$,*

$$\tilde{\Phi}_\epsilon(\mathbf{m}) \leq \inf_{\mathbf{q} \in \mathcal{Q}} \Psi(\mathbf{q}, \mathbf{m}) + \frac{\epsilon}{2}.$$

Proof. Fix any $\mathbf{m} \in \mathcal{L}$ and $\mathbf{q} \in \mathcal{Q}$. For $0 \leq t \leq 1$, define now the interpolating Hamiltonian

$$\begin{aligned} \tilde{H}_t(G; G_*, Z) &= \sum_{1 \leq i < j \leq N} -\frac{t}{2N} \|\phi_i \bullet \phi_j\|_{\mathcal{K}}^2 + \frac{t}{N} \langle \phi_i \bullet \phi_j, \phi_{*i} \bullet \phi_{*j} \rangle_{\mathcal{K}} + \sqrt{\frac{t}{N}} \langle \phi_i \bullet \phi_j, \mathbf{z}_{ij} \rangle_{\mathcal{H}} \\ &\quad + \sum_{i=1}^N -\frac{t}{4N} \|\phi_i \bullet \phi_i\|_{\mathcal{K}}^2 + \frac{t}{2N} \langle \phi_i \bullet \phi_i, \phi_{*i} \bullet \phi_{*i} \rangle_{\mathcal{K}} + \sqrt{\frac{t}{2N}} \langle \phi_i \bullet \phi_i, \mathbf{z}_{ii} \rangle_{\mathcal{H}} \\ &\quad + \sum_{i=1}^N -\frac{(1-t)}{2} \|\mathbf{q}^{1/2} \phi_i\|_{\mathcal{H}}^2 + (1-t) \langle \phi_i, \mathbf{m} \phi_{*i} \rangle_{\mathcal{H}} + \sqrt{1-t} \langle \mathbf{q}^{1/2} \phi_i, \mathbf{z}_i \rangle_{\mathcal{H}} \end{aligned}$$

which differs from (53) only by the term $(1-t)\langle\phi_i, \mathbf{m}\phi_{*i}\rangle_{\mathcal{H}}$ in place of $(1-t)\langle\mathbf{q}^{1/2}\phi_i, \mathbf{q}^{1/2}\phi_{*i}\rangle_{\mathcal{H}}$.

Let

$$\tilde{\Phi}_\epsilon(t; \mathbf{m}) = \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \left[\mathbf{1}\{\|Q(G, G_*) - \mathbf{m}\|_{\mathcal{L}}^2 \leq \epsilon\} \exp \tilde{H}_t(G; G_*, Z) \right] \quad (65)$$

and let $\langle f(G) \rangle_t = \frac{\mathbb{E}_G[f(G)\mathbf{1}\{\|Q(G, G_*) - \mathbf{m}\|_{\mathcal{L}}^2 \leq \epsilon\} \exp \tilde{H}_t(G; G_*, Z)]}{\mathbb{E}_G[\mathbf{1}\{\|Q(G, G_*) - \mathbf{m}\|_{\mathcal{L}}^2 \leq \epsilon\} \exp \tilde{H}_t(G; G_*, Z)]}$ be the corresponding Gibbs average. Note that $\tilde{\Phi}_\epsilon(1; \mathbf{m}) = \tilde{\Phi}_\epsilon(\mathbf{m})$, and when $t = 0$ we have the trivial bound analogous to (55)

$$\tilde{\Phi}_\epsilon(0; \mathbf{m}) \leq \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp \tilde{H}_0(G; G_*, Z) = \Psi(\mathbf{q}, \mathbf{m}) - \frac{1}{4}\|\mathbf{q}\|_{\mathcal{L}}^2 + \frac{1}{2}\|\mathbf{m}\|_{\mathcal{L}}^2.$$

Applying the same calculation as in the proof of Proposition A.2, we have also analogous to (57) that

$$\begin{aligned} \tilde{\Phi}'_\epsilon(t; \mathbf{m}) &= \mathbb{E}_{G_*, Z} \left\langle \frac{1}{2}\|Q(G, G_*)\|_{\mathcal{L}}^2 - \frac{1}{4}\|Q(G, G')\|_{\mathcal{L}}^2 - \langle \mathbf{m}, Q(G, G_*) \rangle_{\mathcal{L}} + \frac{1}{2}\langle \mathbf{q}, Q(G, G') \rangle_{\mathcal{L}} \right\rangle_t \\ &= -\frac{1}{4}\mathbb{E}_{G_*, Z} \langle \|Q(G, G') - \mathbf{q}\|_{\mathcal{L}}^2 \rangle_t + \frac{1}{2}\mathbb{E}_{G_*, Z} \langle \|Q(G, G_*) - \mathbf{m}\|_{\mathcal{L}}^2 \rangle_t + \frac{1}{4}\|\mathbf{q}\|_{\mathcal{L}}^2 - \frac{1}{2}\|\mathbf{m}\|_{\mathcal{L}}^2. \end{aligned}$$

Upper bounding the first negative term by 0 and applying $\|Q(G, G_*) - \mathbf{m}\|_{\mathcal{L}}^2 \leq \epsilon$ with probability 1 under the Gibbs measure defining $\langle \cdot \rangle_t$, we obtain

$$\tilde{\Phi}'_\epsilon(t; \mathbf{m}) \leq \frac{1}{4}\|\mathbf{q}\|_{\mathcal{L}}^2 - \frac{1}{2}\|\mathbf{m}\|_{\mathcal{L}}^2 + \frac{\epsilon}{2}.$$

Thus $\Phi_\epsilon(\mathbf{m}) = \tilde{\Phi}_\epsilon(0; \mathbf{m}) + \int_0^1 \tilde{\Phi}'_\epsilon(t; \mathbf{m}) dt \leq \Psi(\mathbf{q}, \mathbf{m}) + \epsilon/2$, and the lemma follows upon taking the infimum over $\mathbf{q} \in \mathcal{Q}$. \square

Finally, appealing to the closure properties of Assumption 2.1(c), denote by $|\mathbf{m}|, |\mathbf{m}^\top| \in \mathcal{Q}$ the elements for which $\iota(|\mathbf{m}|)^2 = \iota(\mathbf{m})^\top \iota(\mathbf{m})$ and $\iota(|\mathbf{m}^\top|)^2 = \iota(\mathbf{m}) \iota(\mathbf{m})^\top$. The following lemma will allow us to pass the maximization over $\mathbf{m} \in \mathcal{L}$ to $|\mathbf{m}| \in \mathcal{Q}$.

Lemma A.6. *For any $\mathbf{m} \in \mathcal{L}$,*

$$\Psi(|\mathbf{m}^\top|, \mathbf{m}) \leq \Psi(|\mathbf{m}|, |\mathbf{m}|).$$

Proof. Consider the linear observation model

$$\mathbf{y}_i = A\phi_{*i} + \mathbf{z}_i \text{ for } i = 1, \dots, N$$

indexed by a parameter $A \in B(\mathcal{H})$, where $\phi_{*i} = \phi(G_*)_i$, $G_* \sim \text{Haar}(\mathcal{G}_N)$, and $\{\mathbf{z}_i\}_{i=1}^N$ are i.i.d. standard Gaussian noise vectors in \mathcal{H} . Writing $\phi_i = \phi(G)_i$, the marginal log-likelihood of $Y_{\text{lin}} = \{\mathbf{y}_i\}_{i=1}^N$ is given by

$$\log p_A(Y_{\text{lin}}) = \log \mathbb{E}_G \exp \left(-\frac{1}{2} \sum_{i=1}^N \langle A\phi_i, A\phi_i \rangle_{\mathcal{H}} + \sum_{i=1}^N \langle A\phi_i, \mathbf{y}_i \rangle_{\mathcal{H}} \right) - \frac{1}{2} \sum_{i=1}^N \|\mathbf{y}_i\|_{\mathcal{H}}^2 - \frac{N \dim(\mathcal{H})}{2} \log 2\pi.$$

Then for $A, B \in B(\mathcal{H})$, the Kullback-Liebler divergence in this model is

$$\begin{aligned} D_{\text{KL}}(p_A \| p_B) &:= \mathbb{E}_{Y_{\text{lin}} \sim p_A} [\log p_A(Y_{\text{lin}}) - \log p_B(Y_{\text{lin}})] \\ &= \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp \left(-\frac{1}{2} \sum_{i=1}^N \langle A\phi_i, A\phi_i \rangle_{\mathcal{H}} + \sum_{i=1}^N \langle A\phi_i, A\phi_{*i} \rangle_{\mathcal{H}} + \sum_{i=1}^N \langle A\phi_i, \mathbf{z}_i \rangle_{\mathcal{H}} \right) \\ &\quad - \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp \left(-\frac{1}{2} \sum_{i=1}^N \langle B\phi_i, B\phi_i \rangle_{\mathcal{H}} + \sum_{i=1}^N \langle B\phi_i, A\phi_{*i} \rangle_{\mathcal{H}} + \sum_{i=1}^N \langle B\phi_i, \mathbf{z}_i \rangle_{\mathcal{H}} \right) \end{aligned}$$

For any $\mathbf{m} \in \mathcal{L}$, let us write the singular value decomposition $\iota(\mathbf{m}) = UDV^\top$ and specialize the above to $A = \mathbf{m}_V$ and $B = \mathbf{m}_U$ as defined in (17). Then $\iota(\mathbf{m}) = B^\top A$, $\iota(|\mathbf{m}|) = A^\top A$, and $\iota(|\mathbf{m}^\top|) = B^\top B$, so

$$D_{\text{KL}}(p_{\mathbf{m}_V} \| p_{\mathbf{m}_U}) = \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp \left(-\frac{N}{2} \langle |\mathbf{m}|, Q(G, G) \rangle_{\mathcal{L}} + N \langle |\mathbf{m}|, Q(G, G_*) \rangle_{\mathcal{L}} + \sum_{i=1}^N \langle |\mathbf{m}|^{1/2} \phi_i, V^\top \mathbf{z}_i \rangle_{\mathcal{H}} \right) \\ - \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp \left(-\frac{N}{2} \langle |\mathbf{m}^\top|, Q(G, G) \rangle_{\mathcal{L}} + N \langle \mathbf{m}, Q(G, G_*) \rangle_{\mathcal{L}} + \sum_{i=1}^N \langle |\mathbf{m}^\top|^{1/2} \phi_i, U^\top \mathbf{z}_i \rangle_{\mathcal{H}} \right).$$

Applying that $\{V^\top \mathbf{z}_i\}_{i=1}^N$ and $\{U^\top \mathbf{z}_i\}_{i=1}^N$ are both equal in law to $\{\mathbf{z}_i\}_{i=1}^N$, that $Q(G, G) = Q(\text{Id}, \text{Id})$, and that $\|\mathbf{m}\|_{\mathcal{L}}^2 = \|\mathbf{m}\|_{\mathcal{L}}^2 = \|\mathbf{m}^\top\|_{\mathcal{L}}^2$, we get $D_{\text{KL}}(p_{\mathbf{m}_V} \| p_{\mathbf{m}_U}) = \Psi(|\mathbf{m}|, |\mathbf{m}|) - \Psi(|\mathbf{m}^\top|, \mathbf{m})$, and the lemma follows from non-negativity of Kullback–Leibler divergence. \square

Proof of Lemma A.3. Combining Lemmas A.5 and A.6, for any $\mathbf{m} \in \mathcal{L}$ and $\epsilon > 0$,

$$\tilde{\Phi}_\epsilon(\mathbf{m}) \leq \Psi(|\mathbf{m}^\top|, \mathbf{m}) + \frac{\epsilon}{2} \leq \Psi(|\mathbf{m}|, |\mathbf{m}|) + \frac{\epsilon}{2} = \Psi(|\mathbf{m}|) + \frac{\epsilon}{2}.$$

The result follows upon applying this to Lemma A.4, and upper bounding the supremum over $\{|\mathbf{m}| : \mathbf{m} \in \mathcal{L}\}$ by that over $\mathbf{q} \in \mathcal{Q}$. \square

Finally, we conclude the proof of Theorem 2.2 by comparing the perturbed free energy $\tilde{\mathcal{F}}$ with the original free energy \mathcal{F} .

Proof of Theorem 2.2. Define

$$H_t(G; G_*, Z) = H(G; Y) + \sum_{i=1}^N -\frac{t}{4N} \|\phi_i \bullet \phi_i\|_{\mathcal{K}}^2 + \frac{t}{2N} \langle \phi_i \bullet \phi_i, \phi_{*i} \bullet \phi_{*i} \rangle_{\mathcal{K}} + \sqrt{\frac{t}{2N}} \langle \phi_i \bullet \phi_i, \mathbf{z}_{ii} \rangle_{\mathcal{K}},$$

which equals $H(G; Y)$ at $t = 0$ and $\tilde{H}(G; G_*, Z)$ at $t = 1$. Set $\mathcal{F}(t; G_*, Z) = N^{-1} \log \mathbb{E}_G \exp H_t(G; G_*, Z)$, and write $\langle \cdot \rangle_t$ for the average over the corresponding law of G . Then a calculation similar to that in Proposition A.2 using Gaussian integration-by-parts (omitted for brevity) shows, for any fixed $G_* \in \mathcal{G}_N$,

$$\mathbb{E}_Z \mathcal{F}'(t; G_*, Z) = \mathbb{E}_Z \left[\frac{1}{2N^2} \sum_{i=1}^N \left\langle \langle \phi_i \bullet \phi_i \rangle_t, \phi_{*i} \bullet \phi_{*i} \right\rangle_{\mathcal{K}} - \frac{1}{4N^2} \sum_{i=1}^N \left\| \langle \phi_i \bullet \phi_i \rangle_t \right\|_{\mathcal{K}}^2 \right].$$

Recalling $K(\mathcal{G}_N)$ in (10), this implies $|\mathbb{E}_Z \mathcal{F}'(t; G_*, Z)| \leq 3K(\mathcal{G}_N)/(4N)$ for all $t \in [0, 1]$. Then, denoting $\mathcal{F}(G_*, Z) = \mathcal{F}(0; G_*, Z)$ and $\tilde{\mathcal{F}}(G_*, Z) = \mathcal{F}(1; G_*, Z)$ and integrating over $t \in [0, 1]$, we have

$$|\mathbb{E}_Z \mathcal{F}(G_*, Z) - \mathbb{E}_Z \tilde{\mathcal{F}}(G_*, Z)| \leq 3K(\mathcal{G}_N)/(4N). \quad (66)$$

Then also $|\mathcal{F} - \tilde{\mathcal{F}}| = |\mathbb{E}_{G_*, Z} \mathcal{F}(G_*, Z) - \mathbb{E}_{G_*, Z} \tilde{\mathcal{F}}(G_*, Z)| \leq 3K(\mathcal{G}_N)/4N$, and combining with Lemmas A.1 and A.3 concludes the proof. \square

A.3 Overlap concentration

Proof of Corollary 2.3. Define the restricted free energy

$$\tilde{\Phi}_\epsilon = \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \left[\mathbf{1} \{ \|Q(G, G_*) - \mathcal{L}_*(\epsilon)\|_{\mathcal{L}}^2 > \epsilon \} \exp \tilde{H}(G; G_*, Z) \right].$$

Recall the $\sqrt{\epsilon}$ -cover \mathcal{M} from the proof of Lemma A.4. If $\|Q(G, G_*) - \mathcal{L}_*(\epsilon)\|_{\mathcal{L}}^2 > \epsilon$, then the point $\mathbf{m} \in \mathcal{M}$ for which $\|Q(G, G_*) - \mathbf{m}\|_{\mathcal{L}} \leq \sqrt{\epsilon}$ must not belong to $\mathcal{L}_*(\epsilon)$, hence

$$\mathbf{1}\{\|Q(G, G_*) - \mathcal{L}_*(\epsilon)\|_{\mathcal{L}}^2 > \epsilon\} \leq \sum_{\mathbf{m} \in \mathcal{M} \setminus \mathcal{L}_*(\epsilon)} \mathbf{1}\{\|Q(G, G_*) - \mathbf{m}\|_{\mathcal{L}}^2 \leq \epsilon\}.$$

Then the same argument as that of Lemma A.4 shows

$$\tilde{\Phi}_\epsilon \leq \sup_{\mathbf{m} \in \mathcal{L} \setminus \mathcal{L}_*(\epsilon)} \tilde{\Phi}_\epsilon(\mathbf{m}) + D(\mathcal{G}_N) \sqrt{\frac{L(\epsilon^{1/2}; \mathcal{G}_N)}{N}} + \frac{L(\epsilon^{1/2}; \mathcal{G}_N)}{N}.$$

By Lemma A.5 and the argument in Lemma A.6,

$$\tilde{\Phi}_\epsilon(\mathbf{m}) \leq \Psi(|\mathbf{m}^\top|, \mathbf{m}) + \frac{\epsilon}{2} \leq \Psi(|\mathbf{m}|) - D_{\text{KL}}(p_{\mathbf{m}_V} \| p_{\mathbf{m}_U}) + \frac{\epsilon}{2}.$$

If $\mathbf{m} \notin \mathcal{L}_*(\epsilon)$, then either $\Psi(|\mathbf{m}|) \leq \sup_{\mathbf{q} \in \mathcal{Q}} \Psi(\mathbf{q}) - \epsilon$ or $-D_{\text{KL}}(p_{\mathbf{m}_V} \| p_{\mathbf{m}_U}) \leq -\epsilon$. Hence

$$\tilde{\Phi}_\epsilon \leq \sup_{\mathbf{q} \in \mathcal{Q}} \Psi(\mathbf{q}) - \frac{\epsilon}{2} + D(\mathcal{G}_N) \sqrt{\frac{L(\epsilon^{1/2}; \mathcal{G}_N)}{N}} + \frac{L(\epsilon^{1/2}; \mathcal{G}_N)}{N}. \quad (67)$$

Now recall the original Hamiltonian $H(G; Y)$ from (4), and define

$$\begin{aligned} \tilde{\Phi}_\epsilon(G_*, Z) &= \frac{1}{N} \log \mathbb{E}_G \left[\mathbf{1}\{\|Q(G, G_*) - \mathcal{L}_*(\epsilon)\|_{\mathcal{L}}^2 > \epsilon\} \exp \tilde{H}(G; G_*, Z) \right], \\ \Phi_\epsilon(G_*, Z) &= \frac{1}{N} \log \mathbb{E}_G \left[\mathbf{1}\{\|Q(G, G_*) - \mathcal{L}_*(\epsilon)\|_{\mathcal{L}}^2 > \epsilon\} \exp H(G; Y) \right], \\ \tilde{\mathcal{F}}(G_*, Z) &= \frac{1}{N} \log \mathbb{E}_G \left[\exp \tilde{H}(G; G_*, Z) \right], \\ \mathcal{F}(G_*, Z) &= \frac{1}{N} \log \mathbb{E}_G \left[\exp H(G; Y) \right]. \end{aligned}$$

The same argument as (62) shows that all four quantities are $D(\mathcal{G}_N)/\sqrt{2N}$ -Lipschitz in Z for any fixed $G_* \in \mathcal{G}_N$, the same argument as (66) shows

$$|\mathbb{E}_Z \Phi_\epsilon(G_*, Z) - \mathbb{E}_Z \tilde{\Phi}_\epsilon(G_*, Z)|, |\mathbb{E}_Z \mathcal{F}_\epsilon(G_*, Z) - \mathbb{E}_Z \tilde{\mathcal{F}}_\epsilon(G_*, Z)| \leq \frac{3K(\mathcal{G}_N)}{4N},$$

and the same argument as (64) shows $\mathbb{E}_Z \tilde{\Phi}_\epsilon(G_*, Z) = \tilde{\Phi}_\epsilon$ and $\mathbb{E}_Z \tilde{\mathcal{F}}(G_*, Z) = \tilde{\mathcal{F}}$ for every $G_* \in \mathcal{G}_N$. Then by Gaussian concentration of measure [BLB03, Theorem 5.6], for any $u > 0$,

$$\begin{aligned} \mathbb{P}_{G_*, Z} \left[\Phi_\epsilon(G_*, Z) \geq \tilde{\Phi}_\epsilon + u + \frac{3K(\mathcal{G}_N)}{4N} \right] &\leq \mathbb{P}_{G_*, Z} \left[\tilde{\Phi}_\epsilon(G_*, Z) \geq \mathbb{E}_Z \tilde{\Phi}_\epsilon(G_*, Z) + u \right] \leq \exp \left(-\frac{4Nu^2}{D(\mathcal{G}_N)^2} \right), \\ \mathbb{P}_{G_*, Z} \left[\mathcal{F}(G_*, Z) \leq \tilde{\mathcal{F}} - u - \frac{3K(\mathcal{G}_N)}{4N} \right] &\leq \mathbb{P}_{G_*, Z} \left[\tilde{\mathcal{F}}(G_*, Z) \leq \mathbb{E}_Z \tilde{\mathcal{F}}(G_*, Z) - u \right] \leq \exp \left(-\frac{4Nu^2}{D(\mathcal{G}_N)^2} \right). \end{aligned}$$

Choosing $u = \epsilon/8$, it follows that

$$\begin{aligned} \mathbb{E}_{G_*, Z} \left\langle \mathbf{1}\{\|Q(G, G_*) - \mathcal{L}_*(\epsilon)\|_{\mathcal{L}}^2 > \epsilon\} \right\rangle &= \mathbb{E}_{G_*, Z} \frac{\exp N \Phi_\epsilon(G_*, Z)}{\exp N \mathcal{F}(G_*, Z)} \\ &\leq \exp N \left(\tilde{\Phi}_\epsilon - \tilde{\mathcal{F}} + 2 \left(\frac{\epsilon}{8} + \frac{3K(\mathcal{G}_N)}{4N} \right) \right) + 2 \exp \left(-\frac{N\epsilon^2}{16D(\mathcal{G}_N)^2} \right). \end{aligned}$$

Applying (67) and $-\tilde{\mathcal{F}} \leq -\sup_{\mathbf{q} \in \mathcal{Q}} \Psi(\mathbf{q})$ from Lemma A.1, this gives

$$\begin{aligned} & \mathbb{E}_{G_*, Z} \left\langle \mathbf{1} \{ \|Q(G, G_*) - \mathcal{L}_*(\epsilon)\|_{\mathcal{L}}^2 > \epsilon \} \right\rangle \\ & \leq \exp N \left(-\frac{\epsilon}{4} + D(\mathcal{G}_N) \sqrt{\frac{L(\epsilon^{1/2}; \mathcal{G}_N)}{N}} + \frac{L(\epsilon^{1/2}; \mathcal{G}_N)}{N} + \frac{3K(\mathcal{G}_N)}{2N} \right) + 2 \exp \left(-\frac{N\epsilon^2}{16D(\mathcal{G}_N)^2} \right), \end{aligned}$$

implying the corollary. \square

A.4 Mutual information

We verify the mutual information relations (15) and (16). For (15),

$$\begin{aligned} \frac{1}{N} I(G_*, Y) &= \frac{1}{N} \mathbb{E}_{G_*, Z} \log p(Y | G_*) - \frac{1}{N} \mathbb{E}_{G_*, Z} \log p(Y) \\ &= \frac{1}{N} \mathbb{E}_{G_*, Z} \left[\sum_{i < j} -\frac{1}{2N} \|\mathbf{y}_{ij} - \phi_{*i} \bullet \phi_{*j}\|_{\mathcal{K}}^2 \right] - \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp \left(\sum_{i < j} -\frac{1}{2N} \|\mathbf{y}_{ij} - \phi_i \bullet \phi_j\|_{\mathcal{K}}^2 \right) \\ &= \frac{1}{N} \mathbb{E}_{G_*, Z} \left[\sum_{i < j} -\frac{1}{2N} \|\phi_{*i} \bullet \phi_{*j}\|_{\mathcal{K}}^2 + \frac{1}{N} \langle \mathbf{y}_{ij}, \phi_{*i} \bullet \phi_{*j} \rangle_{\mathcal{K}} \right] - \mathcal{F} \\ &= \frac{1}{2N^2} \mathbb{E}_{G_*} \sum_{i < j} \|\phi_{*i} \bullet \phi_{*j}\|_{\mathcal{K}}^2 - \mathcal{F} = \frac{1}{4N^2} \mathbb{E}_{G_*} \sum_{i, j=1}^N \|\phi_{*i} \bullet \phi_{*j}\|_{\mathcal{K}}^2 - \mathcal{F} + O\left(\frac{K(\mathcal{G}_N)}{N}\right) \\ &= \frac{1}{4} \|Q(\text{Id}, \text{Id})\|_{\mathcal{L}}^2 - \mathcal{F} + O\left(\frac{K(\mathcal{G}_N)}{N}\right). \end{aligned} \tag{68}$$

For (16),

$$\begin{aligned} \frac{1}{N} i(G_*, Y_{\text{lin}}) &= \frac{1}{N} \mathbb{E}_{G_*, Z} \log p(Y_{\text{lin}} | G_*) - \frac{1}{N} \mathbb{E}_{G_*, Z} \log p(Y_{\text{lin}}) \\ &= \frac{1}{N} \mathbb{E}_{G_*, Z} \left[\sum_{i=1}^N -\frac{1}{2} \|\mathbf{y}_i - \mathbf{q}^{1/2} \phi_{*i}\|_{\mathcal{H}}^2 \right] - \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp \left(\sum_{i=1}^N -\frac{1}{2} \|\mathbf{y}_i - \mathbf{q}^{1/2} \phi_i\|_{\mathcal{H}}^2 \right) \\ &= \frac{1}{N} \mathbb{E}_{G_*, Z} \left[\sum_{i=1}^N -\frac{1}{2} \|\mathbf{q}^{1/2} \phi_{*i}\|_{\mathcal{H}}^2 + \langle \mathbf{y}_i, \mathbf{q}^{1/2} \phi_{*i} \rangle_{\mathcal{H}} \right] - \left(\Psi(\mathbf{q}) + \frac{1}{4} \|\mathbf{q}\|_{\mathcal{L}}^2 \right) \\ &= \frac{1}{2N} \mathbb{E}_{G_*} \sum_{i=1}^N \langle \mathbf{q}, \phi_{*i} \otimes \phi_{*i} \rangle_{\mathcal{L}} - \left(\Psi(\mathbf{q}) + \frac{1}{4} \|\mathbf{q}\|_{\mathcal{L}}^2 \right) = -\frac{1}{4} \|\mathbf{q}\|_{\mathcal{L}}^2 + \frac{1}{2} \langle \mathbf{q}, Q(\text{Id}, \text{Id}) \rangle_{\mathcal{L}} - \Psi(\mathbf{q}). \end{aligned}$$

B Proofs for group synchronization

B.1 Asymptotic mutual information and MMSE

Proof of Theorem 3.1. Define $\mathcal{G}_N = \mathcal{G}^N$, $\mathcal{H} = \mathcal{K} = \mathcal{L} = \prod_{\ell=1}^L \mathbb{R}^{k_\ell \times k_\ell}$, the feature map $\phi : \mathcal{G}^N \rightarrow \mathcal{H}^N$ by (22), and the bilinear maps \bullet, \otimes and inclusion map ι by (23). We check the conditions of Assumption 2.1:

The compatibility relation (6) follows from

$$\langle \mathbf{a} \bullet \mathbf{b}, \mathbf{a}' \bullet \mathbf{b}' \rangle_{\mathcal{K}} = \sum_{\ell=1}^L \lambda_{\ell} \text{Tr}(\mathbf{a}_{\ell} \mathbf{b}_{\ell}^{\top})^{\top} (\mathbf{a}'_{\ell} \mathbf{b}'_{\ell}{}^{\top}) = \sum_{\ell=1}^L \lambda_{\ell} \text{Tr}(\mathbf{a}_{\ell}^{\top} \mathbf{a}'_{\ell})^{\top} (\mathbf{b}_{\ell}^{\top} \mathbf{b}'_{\ell}) = \langle \mathbf{a} \otimes \mathbf{a}', \mathbf{b} \otimes \mathbf{b}' \rangle_{\mathcal{L}}$$

for all $\mathbf{a}, \mathbf{a}', \mathbf{b}, \mathbf{b}' \in \mathcal{H}$. The inclusion relation (7) follows from

$$\langle \mathbf{a}, \iota(\mathbf{q})\mathbf{b} \rangle_{\mathcal{H}} = \sum_{\ell=1}^L \text{Tr} \mathbf{a}_{\ell}^{\top} (\sqrt{\lambda_{\ell}} \mathbf{b}_{\ell} \mathbf{q}_{\ell}^{\top}) = \sum_{\ell=1}^L \sqrt{\lambda_{\ell}} \text{Tr} \mathbf{q}_{\ell}^{\top} \mathbf{a}_{\ell}^{\top} \mathbf{b}_{\ell} = \langle \mathbf{q}, \mathbf{a} \otimes \mathbf{b} \rangle_{\mathcal{L}}.$$

From this form, we see that $\langle \mathbf{a}, \iota(\mathbf{q})\mathbf{b} \rangle_{\mathcal{H}} = \langle \mathbf{b}, \iota(\mathbf{q})\mathbf{a} \rangle_{\mathcal{H}}$ and $\langle \mathbf{a}, \iota(\mathbf{q})\mathbf{a} \rangle_{\mathcal{H}} \geq 0$ for all $\mathbf{a}, \mathbf{b} \in \mathcal{H}$ if and only if, for every $\ell = 1, \dots, L$, we have $\text{Tr} \mathbf{q}_{\ell}^{\top} \mathbf{m}_{\ell} = \text{Tr} \mathbf{q}_{\ell}^{\top} \mathbf{m}_{\ell}^{\top}$ for all $\mathbf{m}_{\ell} \in \mathbb{R}^{k_{\ell} \times k_{\ell}}$ and $\text{Tr} \mathbf{q}_{\ell}^{\top} \mathbf{m}_{\ell} \geq 0$ for all $\mathbf{m}_{\ell} \in \text{Sym}_{\geq 0}^{k_{\ell} \times k_{\ell}}$, i.e. if and only if each \mathbf{q}_{ℓ} is symmetric positive-semidefinite. Thus the set \mathcal{Q} in (12) is

$$\mathcal{Q} = \text{Sym}_{\geq 0} := \prod_{\ell=1}^L \text{Sym}_{\geq 0}^{k_{\ell} \times k_{\ell}}.$$

Let us write the shorthands

$$I = (I_{k_{\ell} \times k_{\ell}})_{\ell=1}^L, \quad \mathbf{m}^{\top} = (\mathbf{m}_{\ell}^{\top})_{\ell=1}^L, \quad \mathbf{m} \mathbf{m}' = (\mathbf{m}_{\ell} \mathbf{m}'_{\ell})_{\ell=1}^L \text{ for any } \mathbf{m}, \mathbf{m}' \in \mathcal{L}.$$

Note then that inclusion map ι in (23) satisfies $\iota(\mathbf{m})^{\top} = \iota(\mathbf{m}^{\top})$ and $\iota(I)\iota(\mathbf{m} \mathbf{m}') = \iota(\mathbf{m})\iota(\mathbf{m}')$. For any $\mathbf{m} \in \mathcal{L}$, defining $|\mathbf{m}| = ((\mathbf{m}_{\ell}^{\top} \mathbf{m}_{\ell})^{1/2})_{\ell=1}^L \in \mathcal{Q}$ and $|\mathbf{m}^{\top}| = ((\mathbf{m}_{\ell} \mathbf{m}_{\ell}^{\top})^{1/2})_{\ell=1}^L \in \mathcal{Q}$, we then have $\iota(\mathbf{m})^{\top} \iota(\mathbf{m}) = \iota(I)\iota(\mathbf{m}^{\top} \mathbf{m}) = \iota(|\mathbf{m}|)\iota(|\mathbf{m}|)$ and similarly $\iota(\mathbf{m})\iota(\mathbf{m})^{\top} = \iota(|\mathbf{m}^{\top}|)\iota(|\mathbf{m}^{\top}|)$. Furthermore $\|\mathbf{m}_{\ell}\|_F^2 = \||\mathbf{m}|_{\ell}\|_F^2 = \||\mathbf{m}^{\top}|_{\ell}\|_F^2$, verifying the conditions of (8). Finally, for any $\mathbf{g}, \mathbf{h} \in \mathcal{G}$ and each $\ell = 1, \dots, L$, we have $(\mathbf{h}^{-1} \mathbf{g})_{\ell} = \mathbf{h}_{\ell}^{\top} \mathbf{g}_{\ell}$ since $\mathbf{g} \mapsto \mathbf{g}_{\ell}$ is an orthogonal representation of \mathcal{G} . Hence

$$Q(G, H) = \left(\sqrt{\lambda_{\ell}} \cdot \frac{1}{N} \sum_{i=1}^N \mathbf{g}_{\ell}^{(i)\top} \mathbf{h}_{\ell}^{(i)} \right)_{\ell=1}^L = Q(H^{-1}G, \text{Id}).$$

This verifies all the conditions of Assumption 2.1.

Proof of (a): By the independence of the components $(\mathbf{g}_{*}^{(i)}, \mathbf{z}^{(i)})_{i=1}^N$, the expectation $\mathbb{E}_{\mathbf{g}_{*}, \mathbf{z}}$ in (14) is separable across samples $i = 1, \dots, N$, yielding together with the above definitions that

$$\Psi_N(\mathbf{q}) = \sum_{\ell=1}^L -\frac{1}{4} \|\mathbf{q}_{\ell}\|_F^2 - \frac{\sqrt{\lambda_{\ell}}}{2} \text{Tr} \mathbf{q}_{\ell} + \mathbb{E}_{\mathbf{g}_{*}, \mathbf{z}} \log \mathbb{E}_{\mathbf{g}} \exp \left(\sqrt{\lambda_{\ell}} \text{Tr} \mathbf{q}_{\ell} \mathbf{g}_{\ell}^{\top} \mathbf{g}_{* \ell} + \lambda_{\ell}^{1/4} \mathbf{q}_{\ell}^{1/2} \mathbf{g}_{\ell}^{\top} \mathbf{z}_{\ell} \right).$$

In particular, $\Psi_N(\mathbf{q})$ does not depend on N . Defining the change of variables $\mathbf{q}_{\ell} = \sqrt{\lambda_{\ell}} \tilde{\mathbf{q}}_{\ell}$, we then have $\Psi_N(\mathbf{q}) = \Psi_{\text{gs}}(\tilde{\mathbf{q}})$. The quantities $K(\mathcal{G}_N)$, $D(\mathcal{G}_N)$, and $L(\sqrt{\epsilon}; \mathcal{G}_N)$ for any fixed $\epsilon > 0$ are bounded by constants independent of N , so Theorem 2.2 implies

$$\lim_{N \rightarrow \infty} \mathcal{F}_N = \sup_{\mathbf{q} \in \mathcal{Q}} \Psi_N(\mathbf{q}) = \sup_{\tilde{\mathbf{q}} \in \mathcal{Q}} \Psi_{\text{gs}}(\tilde{\mathbf{q}}).$$

Part (a) of the theorem then follows from (15), where $\|Q(\text{Id}, \text{Id})\|_{\mathcal{L}}^2 = \sum_{\ell=1}^L \|\sqrt{\lambda_{\ell}} I_{k_{\ell} \times k_{\ell}}\|_F^2 = \sum_{\ell=1}^L \lambda_{\ell} k_{\ell}$.

Proof of (b): The following I-MMSE relation is standard and follows from similar arguments as in [GSV05], but we include a brief proof for convenience. From (4) and (15), we have

$$\begin{aligned} H(G; G_*, Z) &= -\frac{1}{2N} \sum_{i < j} \sum_{\ell=1}^L \lambda_\ell \|\mathbf{g}_\ell^{(i)} \mathbf{g}_\ell^{(j)\top}\|_F^2 + \frac{1}{N} \sum_{i < j} \sum_{\ell=1}^L \lambda_\ell \text{Tr}(\mathbf{g}_\ell^{(i)} \mathbf{g}_\ell^{(j)\top})^\top (\mathbf{g}_{*\ell}^{(i)} \mathbf{g}_{*\ell}^{(j)\top}) \\ &\quad + \frac{1}{\sqrt{N}} \sum_{i < j} \sum_{\ell=1}^L \sqrt{\lambda_\ell} \text{Tr}(\mathbf{g}_\ell^{(i)} \mathbf{g}_\ell^{(j)\top})^\top \mathbf{z}_\ell^{(ij)}, \\ \frac{1}{N} I(G_*, Y) &= \sum_{\ell=1}^L \frac{\lambda_\ell k_\ell}{4} - \frac{1}{N} \mathbb{E}_{G_*, Z} \log \mathbb{E}_G \exp H(G; G_*, Z). \end{aligned}$$

Taking the derivative with respect to λ_ℓ and applying Gaussian integration-by-parts gives

$$\begin{aligned} \partial_{\lambda_\ell} \frac{1}{N} I(G_*, Y) &= \frac{k_\ell}{4} - \frac{1}{N} \mathbb{E}_{G_*, Z} \left\langle -\frac{1}{2N} \sum_{i < j} \|\mathbf{g}_\ell^{(i)} \mathbf{g}_\ell^{(j)\top}\|_F^2 + \frac{1}{N} \sum_{i < j} \text{Tr}(\mathbf{g}_\ell^{(i)} \mathbf{g}_\ell^{(j)\top})^\top (\mathbf{g}_{*\ell}^{(i)} \mathbf{g}_{*\ell}^{(j)\top}) \right. \\ &\quad \left. + \frac{1}{2\sqrt{\lambda_\ell N}} \sum_{i < j} \text{Tr}(\mathbf{g}_\ell^{(i)} \mathbf{g}_\ell^{(j)\top})^\top \mathbf{z}_\ell^{(ij)} \right\rangle \\ &= \frac{k_\ell}{4} - \frac{1}{N} \mathbb{E}_{G_*, Z} \left[\frac{1}{N} \sum_{i < j} \text{Tr}(\mathbf{g}_\ell^{(i)} \mathbf{g}_\ell^{(j)\top})^\top \mathbf{g}_{*\ell}^{(i)} \mathbf{g}_{*\ell}^{(j)\top} - \frac{1}{2N} \sum_{i < j} \|\langle \mathbf{g}_\ell^{(i)} \mathbf{g}_\ell^{(j)\top} \rangle\|_F^2 \right]. \end{aligned}$$

Then, completing the square and applying $\|\mathbf{g}_{*\ell}^{(i)} \mathbf{g}_{*\ell}^{(j)\top}\|_F^2 = k_\ell$, we obtain the desired I-MMSE relation

$$\partial_{\lambda_\ell} \frac{1}{N} I(G_*, Y) = \frac{1}{2N^2} \sum_{i < j} \mathbb{E}_{G_*, Z} \|\mathbf{g}_{*\ell}^{(i)} \mathbf{g}_{*\ell}^{(j)\top} - \langle \mathbf{g}_\ell^{(i)} \mathbf{g}_\ell^{(j)\top} \rangle\|_F^2 + \frac{k_\ell}{4N} = \frac{1 - N^{-1}}{4} \text{MMSE}_\ell + \frac{k_\ell}{4N}.$$

Fixing any $\{\lambda_{\ell'} : \ell' \neq \ell\}$, observe by properties of conditional expectation that MMSE_ℓ is non-increasing in λ_ℓ , so this I-MMSE relation implies $\lambda_\ell \mapsto -\frac{1}{N} I(G_*, Y)$ is convex. Then its pointwise limit

$$\mathcal{I}(\lambda_\ell) := \lim_{N \rightarrow \infty} -\frac{1}{N} I(G_*, Y) = \sup_{\mathbf{q} \in \text{Sym}_{\geq 0}} \Psi_{\text{gs}}(\mathbf{q}) - \sum_{\ell'=1}^L \frac{\lambda_{\ell'} k_{\ell'}}{4}$$

is also convex, the set $D \subseteq (0, \infty)$ where $\mathcal{I}(\cdot)$ is differentiable has full Lebesgue measure, and for all $\lambda_\ell \in D$ we have $\lim_{N \rightarrow \infty} \partial_{\lambda_\ell} [-\frac{1}{N} I(G_*, Y)] = \mathcal{I}'(\lambda_\ell)$ [Roc15, Theorems 10.8, 24.6, 25.3]. Applying a change of variables $\mathbf{m} = (\lambda_\ell \mathbf{q}_\ell)_{\ell=1}^L$, we may express

$$\mathcal{I}(\lambda_\ell) = \sup_{\mathbf{m} \in \text{Sym}_{\geq 0}} \mathcal{I}(\lambda_\ell, \mathbf{m}), \quad \mathcal{I}(\lambda_\ell, \mathbf{m}) := \sum_{\ell'=1}^L \left(-\frac{\lambda_{\ell'} k_{\ell'}}{4} - \frac{1}{4\lambda_{\ell'}} \|\mathbf{m}_{\ell'}\|_F^2 \right) + F(\mathbf{m})$$

for a function $F(\mathbf{m})$ not depending on λ_ℓ . It may be checked (via the gradient calculation in Proposition 3.2) that this function $F(\mathbf{m})$ is Lipschitz in \mathbf{m} , and hence for any fixed and bounded range of values $\lambda_\ell > 0$ the supremum $\sup_{\mathbf{m} \in \text{Sym}_{\geq 0}} \mathcal{I}(\lambda_\ell, \mathbf{m})$ is attained on a compact subset of $\text{Sym}_{\geq 0}$. Then by the envelope theorem [MS02, Corollary 4], D is precisely the set where $\partial_{\lambda_\ell} \mathcal{I}(\lambda_\ell, \mathbf{m}_*) = -\frac{k_\ell}{4} + \frac{1}{4\lambda_\ell^2} \|\mathbf{m}_{*\ell}\|_F^2$ takes the same value for all $\mathbf{m}_* \in \arg \max_{\mathbf{m} \in \text{Sym}_{\geq 0}} \mathcal{I}(\lambda_\ell, \mathbf{m})$, and $\mathcal{I}'(\lambda_\ell) = -\frac{k_\ell}{4} + \frac{1}{4\lambda_\ell^2} \|\mathbf{m}_{*\ell}\|_F^2$ for any such \mathbf{m}_* . Restating this in terms

of the original variable \mathbf{q} , D is the set where $\|\mathbf{q}_{*\ell}\|_F^2$ takes the same value for all $\mathbf{q}_* \in \arg \max_{\mathbf{q} \in \text{Sym}_{\geq 0}} \Psi_{\text{gs}}(\mathbf{q})$, and for any $\lambda_\ell \in D$ we have

$$\lim_{N \rightarrow \infty} \text{MMSE}_\ell = 4 \lim_{N \rightarrow \infty} \partial_{\lambda_\ell} \frac{1}{N} I(G_*, Y) = -4\mathcal{I}'(\lambda_\ell) = k_\ell - \|\mathbf{q}_{*\ell}\|_F^2,$$

showing part (b).

Proof of (c): We apply Corollary 2.3. Consider any $\mathbf{m} \in \mathcal{L}$, and write the singular value decompositions $\mathbf{m}_\ell = \mathbf{u}_\ell \mathbf{d}_\ell \mathbf{v}_\ell^\top \in \mathbb{R}^{k_\ell \times k_\ell}$. Then $\iota(\mathbf{m})$ admits a singular value decomposition $\iota(\mathbf{m}) = UDV^\top$ where $U, V, D \in B(\mathcal{H})$ are orthogonal and diagonal linear operators defined by

$$U\mathbf{a} = (\mathbf{a}_\ell \mathbf{u}_\ell^\top)_{\ell=1}^L, \quad V\mathbf{a} = (\mathbf{a}_\ell \mathbf{v}_\ell^\top)_{\ell=1}^L, \quad D\mathbf{a} = (\sqrt{\lambda_\ell} \mathbf{a}_\ell \mathbf{d}_\ell)_{\ell=1}^L.$$

So $\mathbf{m}_U, \mathbf{m}_V \in B(\mathcal{H})$ are given by $\mathbf{m}_U \mathbf{a} = (\lambda_\ell^{1/4} \mathbf{a}_\ell \mathbf{u}_\ell \mathbf{d}_\ell^{1/2})_{\ell=1}^L$ and $\mathbf{m}_V \mathbf{a} = (\lambda_\ell^{1/4} \mathbf{a}_\ell \mathbf{v}_\ell \mathbf{d}_\ell^{1/2})_{\ell=1}^L$, and $p_{\mathbf{m}_U}$ is the marginal density of $Y_{\text{lin}} = \{\mathbf{y}_\ell^{(i)}\}_{1 \leq i \leq N, 1 \leq \ell \leq L}$ in the model with observations

$$\mathbf{y}_\ell^{(i)} = \lambda_\ell^{1/4} \mathbf{g}_{*\ell}^{(i)} \mathbf{u}_\ell \mathbf{d}_\ell^{1/2} + \mathbf{z}_\ell^{(i)}.$$

By independence of components for $i = 1, \dots, N$, $\frac{1}{N} D_{\text{KL}}(p_{\mathbf{m}_V} \| p_{\mathbf{m}_U})$ is equal to the Kullback-Liebler divergence between the $N = 1$ models

$$\{\mathbf{y}_\ell = \lambda_\ell^{1/4} \mathbf{g}_{*\ell} \mathbf{v}_\ell \mathbf{d}_\ell^{1/2} + \mathbf{z}_\ell\}_{\ell=1}^L \quad \text{and} \quad \{\mathbf{y}_\ell = \lambda_\ell^{1/4} \mathbf{g}_{*\ell} \mathbf{u}_\ell \mathbf{d}_\ell^{1/2} + \mathbf{z}_\ell\}_{\ell=1}^L.$$

In particular, $\frac{1}{N} D_{\text{KL}}(p_{\mathbf{m}_V} \| p_{\mathbf{m}_U})$ does not depend on N .

Consider $\mathcal{L}_*(0)$ corresponding to (18) with $\epsilon = 0$, and suppose $\mathbf{m} \in \mathcal{L}_*(0)$ where $\mathbf{m}_\ell = \mathbf{u}_\ell \mathbf{d}_\ell \mathbf{v}_\ell^\top$. Then $|\mathbf{m}| = (\mathbf{v}_\ell \mathbf{d}_\ell \mathbf{v}_\ell^\top)_{\ell=1}^L \in \arg \max_{\mathbf{q} \in \mathcal{Q}} \Psi_N(\mathbf{q})$, and also $\frac{1}{N} D_{\text{KL}}(p_{\mathbf{m}_V} \| p_{\mathbf{m}_U}) = 0$. Since $\lambda_\ell > 0$, and the law of any compactly supported random variable $X \in \mathbb{R}^d$ is uniquely determined by that of $X + Z \in \mathbb{R}^d$ when $Z \sim \mathcal{N}(0, I)$, the above characterization of $\frac{1}{N} D_{\text{KL}}(p_{\mathbf{m}_V} \| p_{\mathbf{m}_U})$ implies that $(\mathbf{g}_{*\ell} \mathbf{v}_\ell \mathbf{d}_\ell^{1/2})_{\ell=1}^L$ is equal in law to $(\mathbf{g}_{*\ell} \mathbf{u}_\ell \mathbf{d}_\ell^{1/2})_{\ell=1}^L$. Comparing the supports of these two laws, there must exist $\mathbf{g} \in \mathcal{G}$ for which $(\mathbf{g}_\ell \mathbf{v}_\ell \mathbf{d}_\ell^{1/2})_{\ell=1}^L = (I_{k_\ell \times k_\ell} \mathbf{u}_\ell \mathbf{d}_\ell^{1/2})_{\ell=1}^L$, so $\mathbf{m} = (\mathbf{u}_\ell \mathbf{d}_\ell \mathbf{v}_\ell^\top)_{\ell=1}^L = (\mathbf{g}_\ell \mathbf{v}_\ell \mathbf{d}_\ell \mathbf{v}_\ell^\top)_{\ell=1}^L = \mathbf{g} |\mathbf{m}|$. Thus $\mathcal{L}_*(0) \subseteq \mathcal{S} := \{\mathbf{g} \mathbf{q}_* : \mathbf{g} \in \mathcal{G}, \mathbf{q}_* \in \arg \max_{\mathbf{q} \in \mathcal{Q}} \Psi_N(\mathbf{q})\}$. The reverse inclusion $\mathcal{S} \subseteq \mathcal{L}_*(0)$ is also evident from reversing these arguments. By the relation $\Psi_N(\mathbf{q}) = \Psi_{\text{gs}}(\tilde{\mathbf{q}})$ shown in part (a) where $\mathbf{q}_\ell = \sqrt{\lambda_\ell} \tilde{\mathbf{q}}_\ell$, we have $\mathcal{S} = \{(\sqrt{\lambda_\ell} \mathbf{m}_{*\ell})_{\ell=1}^L : \mathbf{m}_* \in \mathcal{L}_{*,\text{gs}}\}$ for $\mathcal{L}_{*,\text{gs}}$ defined in (31). So this establishes

$$\mathcal{L}_*(0) = \left\{ (\sqrt{\lambda_\ell} \mathbf{m}_{*\ell})_{\ell=1}^L : \mathbf{m}_* \in \mathcal{L}_{*,\text{gs}} \right\}. \quad (69)$$

Since $\Psi_N(|\mathbf{m}|)$ and $\frac{1}{N} D_{\text{KL}}(p_{\mathbf{m}_V} \| p_{\mathbf{m}_U})$ defining $\mathcal{L}_*(\cdot)$ are both independent of N and continuous in \mathbf{m} , for any $\epsilon > 0$, there must exist $\delta := \delta(\epsilon) > 0$ independent of N for which

$$\mathcal{L}_*(\delta) \subseteq \{\mathbf{m} \in \mathcal{L} : \|\mathbf{m} - \mathcal{L}_*(0)\|_{\mathcal{L}}^2 < \epsilon/2\}.$$

Choosing $\delta := \delta(\epsilon)$ sufficiently small, by Corollary 2.3, there then exist constants $C, c > 0$ for which

$$\mathbb{E} \left\langle \mathbf{1} \left\{ \|Q(G, G_*) - \mathcal{L}_*(0)\|_{\mathcal{L}}^2 \geq \epsilon \right\} \right\rangle \leq \mathbb{E} \left\langle \mathbf{1} \left\{ \|Q(G, G_*) - \mathcal{L}_*(\delta)\|_{\mathcal{L}}^2 > \delta \right\} \right\rangle \leq C e^{-cN}$$

Applying $Q(G, G_*) = (\sqrt{\lambda_\ell} \cdot \frac{1}{N} \sum_{i=1}^N \mathbf{g}_\ell^{(i)\top} \mathbf{g}_{*\ell}^{(i)})_{\ell=1}^L$, the characterization of $\mathcal{L}_*(0)$ in (69), and the definition of $\mathcal{L}_{*,\text{gs}}(\epsilon)$ in the theorem statement, we have exactly

$$\left\{ \|Q(G, G_*) - \mathcal{L}_*(0)\|_{\mathcal{L}}^2 \geq \epsilon \right\} = \left\{ \left(\frac{1}{N} \sum_{i=1}^N \mathbf{g}_\ell^{(i)\top} \mathbf{g}_{*\ell}^{(i)} \right)_{\ell=1}^L \notin \mathcal{L}_{*,\text{gs}}(\epsilon) \right\},$$

showing part (c). \square

B.2 Derivatives of the replica potential

Throughout this section, we abbreviate $\langle \cdot \rangle \equiv \langle \cdot \rangle_{\mathbf{q}}$.

Proof of Proposition 3.2. Equip $\text{Sym} = \prod_{\ell=1}^L \text{Sym}^{k_\ell \times k_\ell}$ with the inner-product $\langle \mathbf{a}, \mathbf{b} \rangle \mapsto \sum_{\ell=1}^L \text{Tr } \mathbf{a}_\ell \mathbf{b}_\ell$, and consider the orthonormal basis $\{\mathbf{e}_{ij}^\ell : 1 \leq \ell \leq L, 1 \leq i \leq j \leq k_\ell\}$ of Sym given by

$$\mathbf{e}_{ij}^\ell = \begin{cases} \mathbf{e}_i \mathbf{e}_i^\top & \text{if } i = j \\ \frac{1}{\sqrt{2}} (\mathbf{e}_i \mathbf{e}_j^\top + \mathbf{e}_j \mathbf{e}_i^\top) & \text{if } i < j \end{cases} \quad \text{where } \mathbf{e}_1, \dots, \mathbf{e}_{k_\ell} \text{ are the standard basis vectors in } \mathbb{R}^{k_\ell}.$$

Denote the partial derivatives of a function $f(\cdot)$ in this basis by

$$\partial_{lij} f(\mathbf{q}) = \lim_{\delta \rightarrow 0} \frac{1}{\delta} [f(\mathbf{q}_1, \dots, \mathbf{q}_{\ell-1}, \mathbf{q}_\ell + \delta \mathbf{e}_{ij}^\ell, \mathbf{q}_{\ell+1}, \dots, \mathbf{q}_L) - f(\mathbf{q}_1, \dots, \mathbf{q}_L)].$$

For any \mathbf{q} in the interior of $\text{Sym}_{\geq 0}$, we then have the basis representations

$$\nabla \Psi_{\text{gs}}(\mathbf{q})[\mathbf{x}] = \sum_{\ell=1}^L \sum_{1 \leq i \leq j \leq k_\ell} (\mathbf{x} \cdot \mathbf{e}_{ij}^\ell) \partial_{lij} \Psi_{\text{gs}}(\mathbf{q}), \quad (70)$$

$$\nabla^2 \Psi_{\text{gs}}(\mathbf{q})[\mathbf{x}, \mathbf{x}'] = \sum_{\ell, \ell'=1}^L \sum_{1 \leq i \leq j \leq k_\ell} \sum_{1 \leq i' \leq j' \leq k_{\ell'}} (\mathbf{x} \cdot \mathbf{e}_{ij}^\ell) (\mathbf{x}' \cdot \mathbf{e}_{i'j'}^{\ell'}) \partial_{lij} \partial_{\ell'i'j'} \Psi_{\text{gs}}(\mathbf{q}), \quad (71)$$

so it suffices to compute these first- and second-order partial derivatives of $\Psi_{\text{gs}}(\mathbf{q})$.

Recall that the replica potential is

$$\Psi_{\text{gs}}(\mathbf{q}) = -\frac{1}{4} \sum_{\ell=1}^L \lambda_\ell \|\mathbf{q}_\ell\|_F^2 - \frac{1}{2} \sum_{\ell=1}^L \lambda_\ell \text{Tr } \mathbf{q}_\ell + \mathbb{E}_{\mathbf{g}_*, \mathbf{z}} \log \mathbb{E}_{\mathbf{g}} \exp \left(\sum_{\ell=1}^L \text{Tr} \left(\lambda_\ell \mathbf{q}_\ell \mathbf{g}_{*\ell}^\top + \sqrt{\lambda_\ell} \mathbf{q}_\ell^{1/2} \mathbf{z}_\ell^\top \right) \mathbf{g}_\ell \right).$$

For part (a), consider any \mathbf{q} in the interior of $\text{Sym}_{\geq 0}$. From the definition of ∂_{lij} , we have $\partial_{lij} \mathbf{q}_{\ell'} = 0$ if $\ell \neq \ell'$. For $\ell = \ell'$, we have

$$\partial_{lij} \mathbf{q}_\ell = \mathbf{e}_{ij}^\ell, \quad \partial_{lij} \mathbf{q}_\ell^2 = \mathbf{e}_{ij}^\ell \mathbf{q}_\ell + \mathbf{q}_\ell \mathbf{e}_{ij}^\ell.$$

Noting that $\mathbf{q} \mapsto \mathbf{q}_\ell^{1/2}$ is smooth on the interior of $\text{Sym}_{\geq 0}$, denote its partial derivatives by $\partial_{lij}[\mathbf{q}_\ell^{1/2}]$. Then, applying $\text{Tr } \mathbf{e}_{ij}^\ell = \mathbf{1}\{i = j\}$, we have

$$\partial_{lij} \Psi_{\text{gs}}(\mathbf{q}) = -\frac{\lambda_\ell}{2} \text{Tr } \mathbf{e}_{ij}^\ell \mathbf{q}_\ell - \frac{\lambda_\ell}{2} \mathbf{1}\{i = j\} + \mathbb{E}_{\mathbf{g}_*, \mathbf{z}} \left[\text{Tr} \left(\lambda_\ell \mathbf{e}_{ij}^\ell \mathbf{g}_{*\ell}^\top + \sqrt{\lambda_\ell} \partial_{lij}[\mathbf{q}_\ell^{1/2}] \mathbf{z}_\ell^\top \right) \langle \mathbf{g}_\ell \rangle \right].$$

Setting $f(\mathbf{g}) = \sqrt{\lambda_\ell} \mathbf{g}_\ell \partial_{\ell ij}[\mathbf{q}_\ell^{1/2}] \in \mathbb{R}^{k_\ell \times k_\ell}$ and applying Gaussian integration-by-parts in the form

$$\mathbb{E}_{\mathbf{z}} \text{Tr} \mathbf{z}_\ell^\top \langle f(\mathbf{g}) \rangle = \sum_{i,j=1}^{k_\ell} \mathbb{E}_{\mathbf{z}} \frac{\partial}{\partial z_{\ell ij}} \langle f_{ij}(\mathbf{g}) \rangle = \sqrt{\lambda_\ell} \mathbb{E}_{\mathbf{z}} \text{Tr} \left(\mathbf{q}_\ell^{1/2} \langle \mathbf{g}_\ell^\top f(\mathbf{g}) \rangle - \mathbf{q}_\ell^{1/2} \langle \mathbf{g}_\ell \rangle^\top \langle f(\mathbf{g}) \rangle \right)$$

we obtain

$$\begin{aligned} \partial_{\ell ij} \Psi_{\text{gs}}(\mathbf{q}) &= -\frac{\lambda_\ell}{2} \text{Tr} \mathbf{e}_{ij}^\ell \mathbf{q}_\ell - \frac{\lambda_\ell}{2} \mathbf{1}\{i=j\} + \lambda_\ell \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \text{Tr} \mathbf{e}_{ij}^\ell \mathbf{g}_{*\ell}^\top \langle \mathbf{g}_\ell \rangle \\ &\quad + \lambda_\ell \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \left\langle \text{Tr} \mathbf{q}_\ell^{1/2} \mathbf{g}_\ell^\top \mathbf{g}_\ell \partial_{\ell ij}[\mathbf{q}_\ell^{1/2}] \right\rangle - \lambda_\ell \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \text{Tr} \left[\mathbf{q}_\ell^{1/2} \langle \mathbf{g}_\ell \rangle^\top \langle \mathbf{g}_\ell \rangle \partial_{\ell ij}[\mathbf{q}_\ell^{1/2}] \right]. \end{aligned} \quad (72)$$

Differentiating implicitly $\mathbf{q}_\ell^{1/2} \mathbf{q}_\ell^{1/2} = \mathbf{q}_\ell$ gives $\partial_{\ell ij}[\mathbf{q}_\ell^{1/2}] \mathbf{q}_\ell^{1/2} + \mathbf{q}_\ell^{1/2} \partial_{\ell ij}[\mathbf{q}_\ell^{1/2}] = \mathbf{e}_{ij}^\ell$. Thus, since $\mathbf{q}_\ell^{1/2}$, $\partial_{\ell ij}[\mathbf{q}_\ell^{1/2}]$, and \mathbf{e}_{ij}^ℓ are all symmetric, for any $\mathbf{a} \in \mathbb{R}^{k_\ell \times k_\ell}$ we have

$$\text{Tr} \left(\mathbf{q}_\ell^{1/2} \mathbf{a}^\top \mathbf{a} \partial_{\ell ij}[\mathbf{q}_\ell^{1/2}] \right) = \frac{1}{2} \text{Tr} \left([\partial_{\ell ij}[\mathbf{q}_\ell^{1/2}] \mathbf{q}_\ell^{1/2} + \mathbf{q}_\ell^{1/2} \partial_{\ell ij}[\mathbf{q}_\ell^{1/2}]] \mathbf{a}^\top \mathbf{a} \right) = \frac{1}{2} \text{Tr} \mathbf{e}_{ij}^\ell \mathbf{a}^\top \mathbf{a}. \quad (73)$$

Applying this to (72) and noting that $\mathbf{g}_\ell^\top \mathbf{g}_\ell = I_{k_\ell \times k_\ell}$ because \mathbf{g}_ℓ is orthogonal, the second and fourth terms of (72) cancel and we obtain

$$\partial_{\ell ij} \Psi_{\text{gs}}(\mathbf{q}) = -\frac{\lambda_\ell}{2} \text{Tr} \mathbf{e}_{ij}^\ell \mathbf{q}_\ell + \lambda_\ell \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \text{Tr} \mathbf{e}_{ij}^\ell \mathbf{g}_{*\ell}^\top \langle \mathbf{g}_\ell \rangle - \frac{\lambda_\ell}{2} \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \text{Tr} \mathbf{e}_{ij}^\ell \langle \mathbf{g}_\ell \rangle^\top \langle \mathbf{g}_\ell \rangle.$$

By the Nishimori identity,

$$\mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \text{Tr} \mathbf{e}_{ij}^\ell \mathbf{g}_{*\ell}^\top \langle \mathbf{g}_\ell \rangle = \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \text{Tr} \mathbf{e}_{ij}^\ell \langle \mathbf{g}_\ell \rangle^\top \langle \mathbf{g}_\ell \rangle.$$

Thus

$$\partial_{\ell ij} \Psi_{\text{gs}}(\mathbf{q}) = -\frac{\lambda_\ell}{2} \text{Tr} \mathbf{e}_{ij}^\ell \left(\mathbf{q}_\ell - \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \mathbf{g}_{*\ell}^\top \langle \mathbf{g}_\ell \rangle \right) = -\frac{\lambda_\ell}{2} \text{Tr} \mathbf{e}_{ij}^\ell \left(\mathbf{q}_\ell - \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \langle \mathbf{g}_\ell \rangle^\top \langle \mathbf{g}_\ell \rangle \right).$$

Applying this in (70) and using $\sum_{1 \leq i \leq j \leq k_\ell} (\mathbf{x} \cdot \mathbf{e}_{ij}^\ell) \mathbf{e}_{ij}^\ell = \mathbf{x}_\ell$ gives (32). It is clear that the right side of (32) extends continuously to the boundary of $\text{Sym}_{\geq 0}$, thus establishing (32) for all $\mathbf{q} \in \text{Sym}_{\geq 0}$. Also from this form (32), we have $\nabla \Psi_{\text{gs}}(\mathbf{q}) = 0$, i.e. $\nabla \Psi_{\text{gs}}(\mathbf{q})[\mathbf{x}] = 0$ for all $\mathbf{x} \in \text{Sym}$, if and only if $\mathbf{q}_\ell = \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \langle \mathbf{g}_\ell \rangle^\top \langle \mathbf{g}_\ell \rangle$ for all $\ell = 1, \dots, L$. This shows all claims of part (a).

For part (b), let us compute the second partial derivatives from the form of the first derivative

$$\partial_{\ell' i' j'} \Psi_{\text{gs}}(\mathbf{q}) = -\frac{\lambda_{\ell'}}{2} \text{Tr} \mathbf{e}_{i' j'}^{\ell'} \left(\mathbf{q}_{\ell'} - \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \mathbf{g}_{*\ell'}^\top \langle \mathbf{g}_{\ell'} \rangle \right).$$

For \mathbf{q} in the interior of $\text{Sym}_{\geq 0}$, taking $\partial_{\ell ij}$ using the orthogonality relation

$$\partial_{\ell ij} \text{Tr} \mathbf{e}_{i' j'}^{\ell'} \mathbf{q}_{\ell'} = \mathbf{1}\{\ell = \ell'\} \text{Tr} \mathbf{e}_{i' j'}^{\ell'} \mathbf{e}_{ij}^\ell = \mathbf{1}\{(\ell, i, j) = (\ell', i', j')\}$$

for the first term, we get

$$\partial_{\ell ij} \partial_{\ell' i' j'} \Psi_{\text{gs}}(\mathbf{q}) = -\frac{\lambda_\ell}{2} \mathbf{1}\{(\ell, i, j) = (\ell', i', j')\} + \frac{\lambda_{\ell'}}{2} \mathbb{E}_{\mathbf{g}_{**}, \mathbf{z}} \text{Tr} \mathbf{e}_{i' j'}^{\ell'} \mathbf{g}_{*\ell'}^\top \partial_{\ell ij} \langle \mathbf{g}_{\ell'} \rangle. \quad (74)$$

Let us abbreviate

$$\mathbf{m}_\ell = \lambda_\ell \mathbf{e}_{ij}^\ell \mathbf{g}_{*\ell}^\top \mathbf{g}_\ell + \sqrt{\lambda_\ell} \partial_{\ell ij}[\mathbf{q}_\ell^{1/2}] \mathbf{z}_\ell^\top \mathbf{g}_\ell,$$

momentarily write \otimes for the usual vector space tensor product (in this calculation only, not to be confused with the bilinear map \otimes in the rest of the paper), and denote the linear maps $(\text{Tr} \otimes \text{id})(\mathbf{a} \otimes \mathbf{b}) = (\text{Tr} \mathbf{a}) \mathbf{b}$ and $(\text{Tr} \otimes \text{Tr})(\mathbf{a} \otimes \mathbf{b}) = (\text{Tr} \mathbf{a})(\text{Tr} \mathbf{b})$. Then

$$\partial_{\ell ij} \langle \mathbf{g}_{\ell'} \rangle = \langle (\text{Tr} \mathbf{m}_{\ell}) \mathbf{g}_{\ell'} \rangle - \langle \text{Tr} \mathbf{m}_{\ell} \rangle \langle \mathbf{g}_{\ell'} \rangle = \text{Tr} \otimes \text{id} \left(\langle \mathbf{m}_{\ell} \otimes \mathbf{g}_{\ell'} \rangle - \langle \mathbf{m}_{\ell} \rangle \otimes \langle \mathbf{g}_{\ell'} \rangle \right). \quad (75)$$

To simplify the contributions from the second term of \mathbf{m}_{ℓ} involving \mathbf{z}_{ℓ} , we apply Gaussian integration-by-parts in the forms

$$\begin{aligned} \mathbb{E}_{\mathbf{z}} \text{Tr} \otimes \text{id} \langle \mathbf{z}_{\ell}^{\top} f(\mathbf{g}_{\ell}) \otimes \mathbf{g}_{\ell'} \rangle &= \mathbb{E}_{\mathbf{z}} \sum_{i,j=1}^{k_{\ell}} \frac{\partial}{\partial z_{\ell ij}} \langle f_{ij}(\mathbf{g}_{\ell}) \mathbf{g}_{\ell'} \rangle \\ &= \sqrt{\lambda_{\ell}} \mathbb{E}_{\mathbf{z}} \text{Tr} \otimes \text{id} \left[\langle \mathbf{q}_{\ell}^{1/2} \mathbf{g}_{\ell}^{\top} f(\mathbf{g}_{\ell}) \otimes \mathbf{g}_{\ell'} \rangle - \langle \mathbf{q}_{\ell}^{1/2} \langle \mathbf{g}_{\ell} \rangle^{\top} f(\mathbf{g}_{\ell}) \otimes \mathbf{g}_{\ell'} \rangle \right], \\ \mathbb{E}_{\mathbf{z}} \text{Tr} \otimes \text{id} \left[\langle \mathbf{z}_{\ell}^{\top} f(\mathbf{g}_{\ell}) \rangle \otimes \langle \mathbf{g}_{\ell'} \rangle \right] &= \mathbb{E}_{\mathbf{z}} \sum_{i,j=1}^{k_{\ell}} \frac{\partial}{\partial z_{\ell ij}} [\langle f_{ij}(\mathbf{g}_{\ell}) \rangle \langle \mathbf{g}_{\ell'} \rangle] \\ &= \sqrt{\lambda_{\ell}} \mathbb{E}_{\mathbf{z}} \text{Tr} \otimes \text{id} \left[\langle \mathbf{q}_{\ell}^{1/2} \mathbf{g}_{\ell}^{\top} f(\mathbf{g}_{\ell}) \rangle \otimes \langle \mathbf{g}_{\ell'} \rangle + \langle \mathbf{q}_{\ell}^{1/2} \mathbf{g}_{\ell}^{\top} \langle f(\mathbf{g}_{\ell}) \rangle \otimes \mathbf{g}_{\ell'} \right. \\ &\quad \left. - 2 \mathbf{q}_{\ell}^{1/2} \langle \mathbf{g}_{\ell} \rangle^{\top} \langle f(\mathbf{g}_{\ell}) \rangle \otimes \langle \mathbf{g}_{\ell'} \rangle \right]. \end{aligned}$$

Setting $f(\mathbf{g}_{\ell}) = \sqrt{\lambda_{\ell}} \mathbf{g}_{\ell} \partial_{\ell ij} [\mathbf{q}_{\ell}^{1/2}]$ as before and taking the difference of the above two expressions,

$$\begin{aligned} &\mathbb{E}_{\mathbf{z}} \text{Tr} \otimes \text{id} \left[\langle \sqrt{\lambda_{\ell}} \mathbf{z}_{\ell}^{\top} \mathbf{g}_{\ell} \partial_{\ell ij} [\mathbf{q}_{\ell}^{1/2}] \otimes \mathbf{g}_{\ell'} \rangle - \langle \sqrt{\lambda_{\ell}} \mathbf{z}_{\ell}^{\top} \mathbf{g}_{\ell} \partial_{\ell ij} [\mathbf{q}_{\ell}^{1/2}] \rangle \otimes \langle \mathbf{g}_{\ell'} \rangle \right] \\ &= \lambda_{\ell} \mathbb{E}_{\mathbf{z}} \text{Tr} \otimes \text{id} \left[\langle \mathbf{q}_{\ell}^{1/2} (\mathbf{g}_{\ell} - \langle \mathbf{g}_{\ell} \rangle)^{\top} (\mathbf{g}_{\ell} - \langle \mathbf{g}_{\ell} \rangle) \partial_{\ell ij} [\mathbf{q}_{\ell}^{1/2}] \otimes \mathbf{g}_{\ell'} \rangle \right. \\ &\quad \left. - \langle \mathbf{q}_{\ell}^{1/2} \mathbf{g}_{\ell}^{\top} \mathbf{g}_{\ell} \partial_{\ell ij} [\mathbf{q}_{\ell}^{1/2}] \rangle \otimes \langle \mathbf{g}_{\ell'} \rangle + \mathbf{q}_{\ell}^{1/2} \langle \mathbf{g}_{\ell} \rangle^{\top} \langle \mathbf{g}_{\ell} \rangle \partial_{\ell ij} [\mathbf{q}_{\ell}^{1/2}] \otimes \langle \mathbf{g}_{\ell'} \rangle \right] \\ &= \frac{\lambda_{\ell}}{2} \mathbb{E}_{\mathbf{z}} \text{Tr} \otimes \text{id} \left[\langle \mathbf{e}_{ij}^{\ell} (\mathbf{g}_{\ell} - \langle \mathbf{g}_{\ell} \rangle)^{\top} (\mathbf{g}_{\ell} - \langle \mathbf{g}_{\ell} \rangle) \otimes \mathbf{g}_{\ell'} \rangle - \langle \mathbf{e}_{ij}^{\ell} \mathbf{g}_{\ell}^{\top} \mathbf{g}_{\ell} \rangle \otimes \langle \mathbf{g}_{\ell'} \rangle + \mathbf{e}_{ij}^{\ell} \langle \mathbf{g}_{\ell} \rangle^{\top} \langle \mathbf{g}_{\ell} \rangle \otimes \langle \mathbf{g}_{\ell'} \rangle \right] \end{aligned}$$

where the last equality applies (73) with $\mathbf{a} \in \{\mathbf{g}_{\ell} - \langle \mathbf{g}_{\ell} \rangle, \mathbf{g}_{\ell}, \langle \mathbf{g}_{\ell} \rangle\}$. Expanding the square in the first term, cancelling the terms involving $\text{Tr} \mathbf{e}_{ij}^{\ell} \mathbf{g}_{\ell}^{\top} \mathbf{g}_{\ell} = \mathbf{1}\{i=j\}$, and applying $\text{Tr} \mathbf{e}_{ij}^{\ell} \langle \mathbf{g}_{\ell} \rangle^{\top} \mathbf{g}_{\ell} = \text{Tr} \mathbf{e}_{ij}^{\ell} \mathbf{g}_{\ell}^{\top} \langle \mathbf{g}_{\ell} \rangle$, we get

$$\begin{aligned} &\mathbb{E}_{\mathbf{z}} \text{Tr} \otimes \text{id} \left[\langle \sqrt{\lambda_{\ell}} \mathbf{z}_{\ell}^{\top} \mathbf{g}_{\ell} \partial_{\ell ij} [\mathbf{q}_{\ell}^{1/2}] \otimes \mathbf{g}_{\ell'} \rangle - \langle \sqrt{\lambda_{\ell}} \mathbf{z}_{\ell}^{\top} \mathbf{g}_{\ell} \partial_{\ell ij} [\mathbf{q}_{\ell}^{1/2}] \rangle \otimes \langle \mathbf{g}_{\ell'} \rangle \right] \\ &= \lambda_{\ell} \mathbb{E}_{\mathbf{z}} \text{Tr} \otimes \text{id} \left[-\langle \mathbf{e}_{ij}^{\ell} \mathbf{g}_{\ell}^{\top} \langle \mathbf{g}_{\ell} \rangle \otimes \mathbf{g}_{\ell'} \rangle + \mathbf{e}_{ij}^{\ell} \langle \mathbf{g}_{\ell} \rangle^{\top} \langle \mathbf{g}_{\ell} \rangle \otimes \langle \mathbf{g}_{\ell'} \rangle \right] \end{aligned}$$

Combining this with the contributions from the first term of \mathbf{m}_{ℓ} and substituting into (75), we arrive at

$$\mathbb{E}_{\mathbf{z}} \partial_{\ell ij} \langle \mathbf{g}_{\ell'} \rangle = \lambda_{\ell} \mathbb{E}_{\mathbf{z}} \text{Tr} \otimes \text{id} \left[\langle \mathbf{e}_{ij}^{\ell} \mathbf{g}_{*\ell}^{\top} \mathbf{g}_{\ell} \otimes \mathbf{g}_{\ell'} \rangle - \mathbf{e}_{ij}^{\ell} \mathbf{g}_{*\ell}^{\top} \langle \mathbf{g}_{\ell} \rangle \otimes \langle \mathbf{g}_{\ell'} \rangle - \langle \mathbf{e}_{ij}^{\ell} \mathbf{g}_{\ell}^{\top} \langle \mathbf{g}_{\ell} \rangle \otimes \mathbf{g}_{\ell'} \rangle + \mathbf{e}_{ij}^{\ell} \langle \mathbf{g}_{\ell} \rangle^{\top} \langle \mathbf{g}_{\ell} \rangle \otimes \langle \mathbf{g}_{\ell'} \rangle \right].$$

Applying this back to (74) and using again $\text{Tr} \mathbf{e}_{ij}^\ell \langle \mathbf{g}_\ell \rangle^\top \mathbf{g}_\ell = \text{Tr} \mathbf{e}_{ij}^\ell \mathbf{g}_\ell^\top \langle \mathbf{g}_\ell \rangle$ and Nishimori's identity,

$$\begin{aligned}
\partial_{\ell ij} \partial_{\ell' i' j'} \Psi_{\mathbf{g}_s}(\mathbf{q}) &= -\frac{\lambda_\ell}{2} \mathbf{1}\{(\ell, i, j) = (\ell', i', j')\} \\
&\quad + \frac{\lambda_\ell \lambda_{\ell'}}{2} \mathbb{E}_{\mathbf{g}_*, \mathbf{z}} \text{Tr} \otimes \text{Tr} \left[\langle \mathbf{e}_{ij}^\ell \mathbf{g}_{*\ell}^\top \mathbf{g}_\ell \otimes \mathbf{e}_{i'j'}^{\ell'} \mathbf{g}_{*\ell'}^\top \mathbf{g}_{\ell'} \rangle - \mathbf{e}_{ij}^\ell \mathbf{g}_{*\ell}^\top \langle \mathbf{g}_\ell \rangle \otimes \mathbf{e}_{i'j'}^{\ell'} \mathbf{g}_{*\ell'}^\top \langle \mathbf{g}_{\ell'} \rangle \right. \\
&\quad \left. - \langle \mathbf{e}_{ij}^\ell \mathbf{g}_\ell \langle \mathbf{g}_\ell^\top \rangle \rangle \otimes \mathbf{e}_{i'j'}^{\ell'} \mathbf{g}_{*\ell'}^\top \langle \mathbf{g}_{\ell'} \rangle + \mathbf{e}_{ij}^\ell \langle \mathbf{g}_\ell \rangle^\top \langle \mathbf{g}_\ell \rangle \otimes \mathbf{e}_{i'j'}^{\ell'} \mathbf{g}_{*\ell'}^\top \langle \mathbf{g}_{\ell'} \rangle \right] \\
&= -\frac{\lambda_\ell}{2} \mathbf{1}\{(\ell, i, j) = (\ell', i', j')\} \\
&\quad + \frac{\lambda_\ell \lambda_{\ell'}}{2} \mathbb{E}_{\mathbf{g}_*, \mathbf{z}} \left[\langle \text{Tr} \mathbf{e}_{ij}^\ell \mathbf{g}_{*\ell}^\top \mathbf{g}_\ell \text{Tr} \mathbf{e}_{i'j'}^{\ell'} \mathbf{g}_{*\ell'}^\top \mathbf{g}_{\ell'} \rangle - 2 \text{Tr} \mathbf{e}_{ij}^\ell \mathbf{g}_{*\ell}^\top \langle \mathbf{g}_\ell \rangle \text{Tr} \mathbf{e}_{i'j'}^{\ell'} \mathbf{g}_{*\ell'}^\top \langle \mathbf{g}_{\ell'} \rangle \right. \\
&\quad \left. + \text{Tr} \mathbf{e}_{ij}^\ell \langle \mathbf{g}_\ell \rangle^\top \langle \mathbf{g}_\ell \rangle \text{Tr} \mathbf{e}_{i'j'}^{\ell'} \langle \mathbf{g}_{\ell'} \rangle^\top \langle \mathbf{g}_{\ell'} \rangle \right].
\end{aligned}$$

Applying this in (71) and using $\sum_{1 \leq i \leq j \leq k_\ell} (\mathbf{x} \cdot \mathbf{e}_{ij}^\ell)(\mathbf{x}' \cdot \mathbf{e}_{ij}^\ell) = \text{Tr} \mathbf{x}_\ell \mathbf{x}'_\ell$, $\sum_{1 \leq i \leq j \leq k_\ell} (\mathbf{x} \cdot \mathbf{e}_{ij}^\ell) \mathbf{e}_{ij}^\ell = \mathbf{x}_\ell$, and the analogous identity for \mathbf{x}' gives (33). Again, the right side of (33) extends continuously to the boundary of $\text{Sym}_{\geq 0}$, establishing (33) for all $\mathbf{q} \in \text{Sym}_{\geq 0}$ and showing part (b). \square

Proof of Proposition 3.3. Let us write \mathbb{E} for the expectation over independent and uniformly random elements $\mathbf{g}, \mathbf{h} \sim \text{Haar}(\mathcal{G})$, with corresponding representations $(\mathbf{g}_1, \dots, \mathbf{g}_L)$ and $(\mathbf{h}_1, \dots, \mathbf{h}_L)$.

We use the definition of the type of a real-irreducible representation \mathbf{g}_ℓ following Theorem D.13. If the representation \mathbf{g}_ℓ is of real type, then it is \mathbb{C} -irreducible. Since it is also non-trivial, Schur orthogonality (Theorem D.7(a)) implies that $\mathbb{E}[g_{\ell ij} \cdot 1] = 0$ for each entry (i, j) of \mathbf{g}_ℓ , where 1 represents the trivial representation in $\mathbb{C}^{1 \times 1}$; thus $\mathbb{E}[\mathbf{g}_\ell] = 0$. If \mathbf{g}_ℓ is of complex or quaternionic type, then the same argument applies to the entries of the two \mathbb{C} -irreducible sub-representations of \mathbf{g}_ℓ . Thus in all cases, $\mathbb{E}[\mathbf{g}_\ell] = 0$.

At $\mathbf{q} = \mathbf{0}$, a sample \mathbf{g} from the posterior measure defining $\langle \cdot \rangle_{\mathbf{g}}$ is uniform over \mathcal{G} and independent of \mathbf{g}_* . Thus

$$\nabla \Psi(\mathbf{0})[\mathbf{x}] = \sum_{\ell=1}^L \frac{\lambda_\ell}{2} \text{Tr} \mathbf{x}_\ell (\mathbb{E} \mathbf{g}_\ell)^\top (\mathbb{E} \mathbf{g}_\ell) = 0$$

for any $\mathbf{x} \in \text{Sym}$, showing the first claim that $\nabla \Psi(\mathbf{0}) = 0$. Furthermore, applying $\mathbb{E} \mathbf{g}_\ell = 0$,

$$\nabla^2 \Psi(\mathbf{0})[\mathbf{x}, \mathbf{x}'] = \sum_{\ell=1}^L -\frac{\lambda_\ell}{2} \text{Tr} \mathbf{x}_\ell \mathbf{x}'_\ell + \sum_{\ell, \ell'=1}^L \frac{\lambda_\ell \lambda_{\ell'}}{2} \mathbb{E} \left[(\text{Tr} \mathbf{x}_\ell \mathbf{g}_\ell^\top \mathbf{h}_\ell) (\text{Tr} \mathbf{x}'_{\ell'} \mathbf{g}_{\ell'}^\top \mathbf{h}_{\ell'}) \right].$$

By invariance of Haar measure, we have the equality in law $\mathbf{g}^\top \mathbf{h} \stackrel{L}{=} \mathbf{g}$. Furthermore, if $\ell \neq \ell'$, then \mathbf{g}_ℓ and $\mathbf{g}_{\ell'}$ are distinct and real-irreducible, so the \mathbb{C} -irreducible sub-representations of \mathbf{g}_ℓ are distinct from those of $\mathbf{g}_{\ell'}$ (c.f. Theorem D.13). Then Schur orthogonality (Theorem D.7(a)) implies $\mathbb{E}[(\text{Tr} \mathbf{x}_\ell \mathbf{g}_\ell) (\text{Tr} \mathbf{x}'_{\ell'} \mathbf{g}_{\ell'})] = 0$. Thus

$$\nabla^2 \Psi(\mathbf{0})[\mathbf{x}, \mathbf{x}'] = \sum_{\ell=1}^L \underbrace{-\frac{\lambda_\ell}{2} \text{Tr} \mathbf{x}_\ell \mathbf{x}'_\ell + \frac{\lambda_\ell^2}{2} \mathbb{E} \left[(\text{Tr} \mathbf{x}_\ell \mathbf{g}_\ell) (\text{Tr} \mathbf{x}'_\ell \mathbf{g}_\ell) \right]}_{=: H_\ell[\mathbf{x}_\ell, \mathbf{x}'_\ell]}$$

This shows that $\nabla^2 \Psi(\mathbf{0})$ is block-diagonal in the $L \times L$ block decomposition with respect to $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_L)$, with blocks $\{H_\ell\}_{\ell=1}^L$, so its largest eigenvalue satisfies

$$\lambda_{\max}(\nabla^2 \Psi(\mathbf{0})) = \max_{\ell=1}^L \lambda_{\max}(H_\ell) = \max_{\ell=1}^L \sup_{\mathbf{x}_\ell \in \text{Sym}^{k_\ell \times k_\ell}; \|\mathbf{x}_\ell\|_F^2 = k_\ell} \frac{1}{k_\ell} H_\ell[\mathbf{x}_\ell, \mathbf{x}_\ell].$$

If \mathbf{g}_ℓ is of real type, then it is \mathbb{C} -irreducible, and Theorem D.7(a) gives

$$\mathbb{E}[(\text{Tr } \mathbf{x}_\ell \mathbf{g}_\ell)^2] = \mathbb{E}[(\text{Tr } \mathbf{x}_\ell \mathbf{g}_\ell)(\text{Tr } \overline{\mathbf{x}_\ell \mathbf{g}_\ell})] = \sum_{i,j,i',j'=1}^{k_\ell} x_{\ell ij} \overline{x_{\ell i'j'}} \mathbb{E}[g_{\ell ij} \overline{g_{\ell i'j'}}] = \frac{1}{k_\ell} \sum_{i,j=1}^{k_\ell} x_{\ell ij} \overline{x_{\ell i'j'}} = \frac{1}{k_\ell} \|\mathbf{x}_\ell\|_F^2.$$

Thus

$$\sup_{\mathbf{x}_\ell: \|\mathbf{x}_\ell\|_F^2 = k_\ell} \mathbb{E}[(\text{Tr } \mathbf{x}_\ell \mathbf{g}_\ell)^2] = \mathbb{E}[(\text{Tr } \mathbf{g}_\ell)^2] = 1$$

where the first equality holds because the supremum is attained at any \mathbf{x}_ℓ satisfying $\|\mathbf{x}_\ell\|_F^2 = k_\ell$, and in particular at $\mathbf{x}_\ell = I_{k_\ell \times k_\ell}$.

If \mathbf{g}_ℓ is of complex type, then there exists a unitary matrix $(\mathbf{v}_1 \ \mathbf{v}_2) \in \mathbb{C}^{k_\ell \times k_\ell}$ for which

$$\mathbf{g}_\ell = (\mathbf{v}_1 \ \mathbf{v}_2) \begin{pmatrix} \mathbf{g}_\ell^{(1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{g}_\ell^{(2)} \end{pmatrix} \begin{pmatrix} \mathbf{v}_1^* \\ \mathbf{v}_2^* \end{pmatrix} \quad (76)$$

and $\mathbf{g}_\ell^{(1)}, \mathbf{g}_\ell^{(2)} \in \mathbb{C}^{k_\ell/2 \times k_\ell/2}$ are the two \mathbb{C} -irreducible unitary sub-representations of \mathbf{g}_ℓ (c.f. Theorem D.5). Here, $\mathbf{g}_\ell^{(2)}$ is distinct from $\mathbf{g}_\ell^{(1)}$ and isomorphic to the complex conjugate representation $\overline{\mathbf{g}_\ell^{(1)}}$. Then Theorem D.7(a) gives, similarly as above,

$$\mathbb{E}[(\text{Tr } \mathbf{x}_\ell \mathbf{g}_\ell)^2] = \mathbb{E}[(\text{Tr } \mathbf{v}_1^* \mathbf{x}_\ell \mathbf{v}_1 \mathbf{g}_\ell^{(1)} + \text{Tr } \mathbf{v}_2^* \mathbf{x}_\ell \mathbf{v}_2 \mathbf{g}_\ell^{(2)})^2] = \frac{1}{k_\ell/2} \|\mathbf{v}_1^* \mathbf{x}_\ell \mathbf{v}_1\|_F^2 + \frac{1}{k_\ell/2} \|\mathbf{v}_2^* \mathbf{x}_\ell \mathbf{v}_2\|_F^2.$$

We have $\|\mathbf{v}_1^* \mathbf{x}_\ell \mathbf{v}_1\|_F^2 + \|\mathbf{v}_2^* \mathbf{x}_\ell \mathbf{v}_2\|_F^2 \leq \|\mathbf{x}_\ell\|_F^2$, where equality is again attained at $\mathbf{x}_\ell = I_{k_\ell \times k_\ell}$. Then

$$\sup_{\mathbf{x}_\ell: \|\mathbf{x}_\ell\|_F^2 = k_\ell} \mathbb{E}[(\text{Tr } \mathbf{x}_\ell \mathbf{g}_\ell)^2] = \mathbb{E}[(\text{Tr } \mathbf{g}_\ell)^2] = 2.$$

Finally, if \mathbf{g}_ℓ is of quaternionic type, then again (76) holds where, now, $\mathbf{g}_\ell^{(1)}, \mathbf{g}_\ell^{(2)}$ are isomorphic \mathbb{C} -irreducible sub-representations of \mathbf{g}_ℓ (and both isomorphic to $\overline{\mathbf{g}_\ell^{(1)}}$). Then there exists a unitary matrix $\mathbf{u} \in \mathbb{C}^{k_\ell/2 \times k_\ell/2}$ for which $\mathbf{g}_\ell^{(1)} = \mathbf{u}^* \mathbf{g}_\ell^{(2)} \mathbf{u}$ (c.f. Proposition D.9). Replacing $(\mathbf{v}_2, \mathbf{g}_\ell^{(2)})$ by $(\mathbf{v}_2 \mathbf{u}, \mathbf{u}^* \mathbf{g}_\ell^{(2)} \mathbf{u})$, we may assume that $\mathbf{g}_\ell^{(1)} = \mathbf{g}_\ell^{(2)}$. Then by Theorem D.7(a),

$$\mathbb{E}[(\text{Tr } \mathbf{x}_\ell \mathbf{g}_\ell)^2] = \mathbb{E}\left[\left(\text{Tr}(\mathbf{v}_1^* \mathbf{x}_\ell \mathbf{v}_1 + \mathbf{v}_2^* \mathbf{x}_\ell \mathbf{v}_2) \mathbf{g}_\ell^{(1)}\right)^2\right] = \frac{1}{k_\ell/2} \|\mathbf{v}_1^* \mathbf{x}_\ell \mathbf{v}_1 + \mathbf{v}_2^* \mathbf{x}_\ell \mathbf{v}_2\|_F^2.$$

We have $\|\mathbf{v}_1^* \mathbf{x}_\ell \mathbf{v}_1 + \mathbf{v}_2^* \mathbf{x}_\ell \mathbf{v}_2\|_F^2 \leq 2\|\mathbf{v}_1^* \mathbf{x}_\ell \mathbf{v}_1\|_F^2 + 2\|\mathbf{v}_2^* \mathbf{x}_\ell \mathbf{v}_2\|_F^2 \leq 2\|\mathbf{x}_\ell\|_F^2$, where both equalities are attained at $\mathbf{x}_\ell = I_{k_\ell \times k_\ell}$ (since then $\mathbf{v}_1^* \mathbf{x}_\ell \mathbf{v}_1 = \mathbf{v}_2^* \mathbf{x}_\ell \mathbf{v}_2 = I_{k_\ell/2 \times k_\ell/2}$). Thus

$$\sup_{\mathbf{x}_\ell: \|\mathbf{x}_\ell\|_F^2 = k_\ell} \mathbb{E}[(\text{Tr } \mathbf{x}_\ell \mathbf{g}_\ell)^2] = \mathbb{E}[(\text{Tr } \mathbf{g}_\ell)^2] = 4.$$

Defining $\rho_\ell := \mathbb{E}[(\text{Tr } \mathbf{g}_\ell)^2]$, this verifies in all cases that

$$\lambda_{\max}(\nabla^2 \Psi(\mathbf{0})) = \max_{\ell=1}^L \lambda_{\max}(H_\ell) = \max_{\ell=1}^L \frac{1}{k_\ell} \left(-\frac{\lambda_\ell}{2} k_\ell + \frac{\lambda_\ell^2}{2} \rho_\ell \right).$$

Then setting $\tilde{\lambda}_\ell = \lambda_\ell \rho_\ell / k_\ell$, we have that $\lambda_{\max}(\nabla^2 \Psi(\mathbf{0})) < 0$ when $\max_\ell \tilde{\lambda}_\ell < 1$, and $\lambda_{\max}(\nabla^2 \Psi(\mathbf{0})) > 0$ when $\max_\ell \tilde{\lambda}_\ell > 1$, as claimed in parts (a) and (b) of the proposition.

Finally, to conclude the statements about $\mathbf{0}$ being a local maximizer of $\Psi(\mathbf{q})$, observe that since $\text{Sym}_{\succeq 0}$ is a (convex) cone, we have

$$B_\epsilon(\mathbf{0}) := \{\mathbf{q} \in \text{Sym}_{\succeq 0} : \|\mathbf{q}\|_F \leq \epsilon\} = \{t\mathbf{x} : \mathbf{x} \in \text{Sym}_{\succeq 0}, \|\mathbf{x}\|_F = 1, t \in [0, \epsilon]\}.$$

For any such $\mathbf{q} = t\mathbf{x} \in B_\epsilon(\mathbf{0})$, Taylor expansion along the line from $\mathbf{0}$ to \mathbf{q} gives

$$\Psi(\mathbf{q}) - \Psi(\mathbf{0}) = \int_0^t \nabla \Psi(s\mathbf{x})[\mathbf{x}] ds = \int_0^t \nabla \Psi(s\mathbf{x})[\mathbf{x}] - \nabla \Psi(\mathbf{0})[\mathbf{x}] ds = \int_{0 \leq r \leq s \leq t} \nabla^2 \Psi(r\mathbf{x})[\mathbf{x}, \mathbf{x}] dr ds$$

where the second equality uses $\nabla \Psi(\mathbf{0}) = 0$. If $\max_\ell \tilde{\lambda}_\ell < 1$, then $\lambda_{\max}(\nabla^2 \Psi(\mathbf{0})) < 0$, so by continuity there is some $\epsilon > 0$ such that $\lambda_{\max}(\nabla^2 \Psi(r\mathbf{x})) \leq -\epsilon$ for all $r\mathbf{x} \in B_\epsilon(\mathbf{0})$. The above then implies $\Psi(\mathbf{q}) < \Psi(\mathbf{0})$ for all $\mathbf{q} \in B_\epsilon(\mathbf{0})$, so $\mathbf{q} = \mathbf{0}$ is a local maximizer of $\Psi(\mathbf{q})$. Conversely, if $\tilde{\lambda}_\ell > 1$ for some ℓ , then choosing $\mathbf{x} \in \text{Sym}_{\succeq 0}$ with $\mathbf{x}_\ell = I_{k_\ell \times k_\ell} / \sqrt{k_\ell}$ and $\mathbf{x}_{\ell'} = \mathbf{0}$ for all $\ell' \neq \ell$, the above proof verifies that $\nabla^2 \Psi(\mathbf{0})[\mathbf{x}, \mathbf{x}] > 0$. Then by continuity, $\nabla^2 \Psi(r\mathbf{x})[\mathbf{x}, \mathbf{x}] > \epsilon > 0$ for some $\epsilon > 0$ and all $r \in [0, \epsilon]$. Then the above shows $\Psi(\mathbf{q}) > \Psi(\mathbf{0})$ for $\mathbf{q} = t\mathbf{x}$ and all $t \in (0, \epsilon)$, so $\mathbf{q} = \mathbf{0}$ is not a local maximizer of $\Psi(\mathbf{q})$. \square

B.3 $\mathbb{S}\mathbb{O}(2)$ -synchronization

We now prove Theorem 3.10, providing a global analysis of the optimization problem $\sup_{\mathbf{q} \in \mathcal{Q}} \Psi_{\text{gs}}(\mathbf{q})$ for the single-channel $\mathbb{S}\mathbb{O}(2)$ -synchronization model.

Proof of Proposition 3.9. If $\mathbf{q} \in \text{Sym}_{\succeq 0}$ is a critical point of Ψ_{gs} , then Proposition 3.2(a) shows $\mathbf{q}_\ell = \mathbb{E} \langle \mathbf{g}_\ell \rangle_{\mathbf{q}}^\top \langle \mathbf{g}_\ell \rangle_{\mathbf{q}}$ for all ℓ . Then \mathbf{q}_ℓ is a symmetric matrix that commutes with \mathbf{h}_ℓ for every $\mathbf{h} \in \mathcal{G}$ because \mathcal{G} is abelian, so it is a multiple of the identity by Schur's lemma (c.f. Theorem D.11).

To establish the result also for local maximizers on the boundary of $\text{Sym}_{\succeq 0}$, consider any $\mathbf{q} \in \text{Sym}_{\succeq 0}$ for which some \mathbf{q}_ℓ is not a multiple of the identity. The above implies $\mathbb{E} \langle \mathbf{g}_\ell \rangle_{\mathbf{q}}^\top \langle \mathbf{g}_\ell \rangle_{\mathbf{q}} = \mu_\ell I$ for some $\mu_\ell \geq 0$. If \mathbf{q}_ℓ has a strictly positive eigenvalue different from μ_ℓ , with eigenvector \mathbf{v}_ℓ , then defining \mathbf{x} by $\mathbf{x}_\ell = \mathbf{v}_\ell \mathbf{v}_\ell^\top$ and $\mathbf{x}_{\ell'} = \mathbf{0}$ for all $\ell' \neq \ell$, Proposition 3.2(a) shows $\nabla \Psi_{\text{gs}}(\mathbf{q})[\mathbf{x}] \neq 0$. Then the point $\mathbf{q}' = \mathbf{q} \pm \epsilon \mathbf{x}$ for some choice of sign \pm and any sufficiently small $\epsilon > 0$ satisfies $\mathbf{q}' \in \text{Sym}_{\succeq 0}$ and $\Psi_{\text{gs}}(\mathbf{q}') > \Psi_{\text{gs}}(\mathbf{q})$. If \mathbf{q}_ℓ does not have a strictly positive eigenvalue different from μ_ℓ , then \mathbf{q}_ℓ must have all eigenvalues equal to 0 and $\mu_\ell \neq 0$. In this case, let \mathbf{v}_ℓ be an eigenvector corresponding to 0, and define \mathbf{x} in the same way. Proposition 3.2(a) shows $\nabla \Psi_{\text{gs}}(\mathbf{q})[\mathbf{x}] > 0$, so the point $\mathbf{q}' = \mathbf{q} + \epsilon \mathbf{x}$ for any sufficiently small $\epsilon > 0$ also satisfies $\mathbf{q}' \in \text{Sym}_{\succeq 0}$ and $\Psi_{\text{gs}}(\mathbf{q}') > \Psi_{\text{gs}}(\mathbf{q})$. In both cases, \mathbf{q} is not a local maximizer of Ψ_{gs} , implying the proposition. \square

To show Theorem 3.10, since $\mathbb{S}\mathbb{O}(2)$ is abelian, Proposition 3.9 allows us to restrict attention to the single-letter model (40) with mean-squared-error function $\text{mmse}(\gamma)$. The main technical lemma is the following.

Lemma B.1. *Let $F(\gamma) = 1 - \frac{1}{2} \text{mmse}(\gamma)$. Then $F(0) = 0$, $F'(0) = 1$, and $F(\gamma)$ is strictly increasing and strictly concave over $\gamma \in (0, \infty)$.*

Proof. It will be convenient to work with the complex variable $u = e^{i\theta} \in \mathbb{U}(1)$ representing

$$\mathbf{g} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \in \mathbb{S}\mathbb{O}(2).$$

Observing \mathbf{y} in the single-letter model (40) is equivalent to observing the sufficient statistic $\sqrt{\gamma}(\cos \theta_*, \sin \theta_*) + (\frac{z_{11} + z_{22}}{2}, \frac{z_{21} - z_{12}}{2})$, which we may represent by the complex observation

$$y = \sqrt{\gamma}u_* + z \in \mathbb{C}$$

where $u_* = e^{i\theta_*} \sim \text{Haar}(\mathbb{U}(1))$ and $\Re z, \Im z \stackrel{iid}{\sim} \mathcal{N}(0, \frac{1}{2})$. Then $p(u | y) \propto e^{-|y - \sqrt{\gamma}u|^2} \propto e^{H(u; y)}$ for the Hamiltonian

$$H(u; y) = \sqrt{\gamma}(y\bar{u} + u\bar{y}) = \gamma(u_*\bar{u} + u\bar{u}_*) + \sqrt{\gamma}(z\bar{u} + u\bar{z}).$$

Abbreviating $\mathbb{E} = \mathbb{E}_{u_*, z}$ and $\langle \cdot \rangle$ for the posterior mean under $p(\cdot | y)$, we have

$$\begin{aligned} \text{mmse}(\gamma) &= \mathbb{E}[2(\cos \theta_* - \langle \cos \theta \rangle)^2 + 2(\sin \theta_* - \langle \sin \theta \rangle)^2] \\ &= 2\mathbb{E}|u_* - \langle u \rangle|^2 = 2(1 - \mathbb{E}\bar{u}_*\langle u \rangle) = 2(1 - \mathbb{E}\langle \bar{u} \rangle \langle u \rangle), \end{aligned}$$

so $F(\gamma) = 1 - \frac{1}{2} \text{mmse}(\gamma) = \mathbb{E}\bar{u}_*\langle u \rangle = \mathbb{E}\langle \bar{u} \rangle \langle u \rangle$. At $\gamma = 0$ we have $\langle u \rangle = 0$, so $F(0) = 0$.

Differentiating in γ and applying the Gaussian integration-by-parts formulas $\mathbb{E}z f(z, \bar{z}) = \mathbb{E}\partial_{\bar{z}} f(z, \bar{z})$ and $\mathbb{E}\bar{z} f(z, \bar{z}) = \mathbb{E}\partial_z f(z, \bar{z})$, we get

$$\begin{aligned} F'(\gamma) &= \mathbb{E}\bar{u}_* \left\langle u \left(u_*\bar{u} + u\bar{u}_* + \frac{1}{2\sqrt{\gamma}}(z\bar{u} + u\bar{z}) \right) \right\rangle - \mathbb{E}\bar{u}_*\langle u \rangle \left\langle u_*\bar{u} + u\bar{u}_* + \frac{1}{2\sqrt{\gamma}}(z\bar{u} + u\bar{z}) \right\rangle \\ &= \mathbb{E} \left[1 - \langle \bar{u} \rangle \langle u \rangle + \bar{u}_*^2(\langle u^2 \rangle - \langle u \rangle^2) + \frac{z\bar{u}_*}{2\sqrt{\gamma}}(1 - \langle \bar{u} \rangle \langle u \rangle) + \frac{\bar{z}u_*}{2\sqrt{\gamma}}(\langle u^2 \rangle - \langle u \rangle^2) \right] \\ &= \mathbb{E} \left[1 - \langle \bar{u} \rangle \langle u \rangle + \bar{u}_*^2(\langle u^2 \rangle - \langle u \rangle^2) + \frac{\bar{u}_*}{2}(-\langle u \rangle - \langle \bar{u} \rangle \langle u^2 \rangle + 2\langle \bar{u} \rangle \langle u \rangle^2) + \frac{\bar{u}_*}{2}(-\langle u \rangle - \langle \bar{u} \rangle \langle u^2 \rangle + 2\langle \bar{u} \rangle \langle u \rangle^2) \right] \\ &= \mathbb{E} \left[1 - \langle \bar{u} \rangle \langle u \rangle + \bar{u}_*^2(\langle u^2 \rangle - \langle u \rangle^2) - \bar{u}_*\langle u \rangle - \bar{u}_*\langle \bar{u} \rangle \langle u^2 \rangle + 2\bar{u}_*\langle \bar{u} \rangle \langle u \rangle^2 \right] \\ &= \mathbb{E} \left[1 - 2\langle \bar{u} \rangle \langle u \rangle + \langle \bar{u} \rangle^2 \langle u \rangle^2 + (\langle \bar{u}^2 \rangle - \langle \bar{u} \rangle^2)(\langle u^2 \rangle - \langle u \rangle^2) \right] \\ &= \mathbb{E} \left[(1 - |\langle u \rangle|^2)^2 + |\langle u^2 \rangle - \langle u \rangle^2|^2 \right]. \end{aligned}$$

Here, both terms are non-negative. For any (finite) $\gamma > 0$ the posterior law of u is not a point mass on the circle $\mathbb{U}(1)$, so $|\langle u \rangle| < 1$ with probability 1 over y . Then the first term is strictly positive, showing that $F(\gamma)$ is strictly increasing. At $\gamma = 0$, we have $\langle u \rangle = \langle u^2 \rangle = 0$, so $F'(0) = 1$.

It remains to show that $F(\gamma)$ is strictly concave. For this, observe first that the Hamiltonian $H(u; y)$ defining the posterior mean $\langle \cdot \rangle$ depends on (γ, y) only via $\sqrt{\gamma}y$. Observe next that by rotational symmetry of the model about the origin in the complex plane, the function $\sqrt{\gamma}y \mapsto (1 - |\langle u \rangle|^2)^2 + |\langle u^2 \rangle - \langle u \rangle^2|^2$ depends only on the modulus $\sqrt{\gamma}|y|$. Thus, setting $x = \sqrt{\gamma}|y|$, we may define

$$f(x) = (1 - |\langle u \rangle|^2)^2 + |\langle u^2 \rangle - \langle u \rangle^2|^2 \text{ where } \langle u^j \rangle = \frac{\mathbb{E}_{u \sim \text{Haar}(\mathbb{U}(1))} u^j e^{x(u + \bar{u})}}{\mathbb{E}_{u \sim \text{Haar}(\mathbb{U}(1))} e^{x(u + \bar{u})}}$$

for real arguments $x \geq 0$, and we have $F'(\gamma) = \mathbb{E}f(\sqrt{\gamma}|y|)$. It then suffices to show

1. For any $\gamma_1 > \gamma_2 > 0$, the law of $x_1 = \sqrt{\gamma_1}|y|$ stochastically dominates that of $x_2 = \sqrt{\gamma_2}|y|$, in the sense $\mathbb{P}[x_1 \geq t] > \mathbb{P}[x_2 \geq t]$ for all $t > 0$.
2. $f'(x) < 0$ for all $x > 0$.

Indeed, then there would exist a coupling of (x_1, x_2) so that $x_1 > x_2$ with probability 1, hence $F'(\gamma_1) - F'(\gamma_2) = \mathbb{E}[f(x_1) - f(x_2)] = \mathbb{E}[\int_{x_2}^{x_1} f'(t)dt] < 0$, implying strictly concavity of $F(\gamma)$.

To show claim (1), observe that $2|y|^2 \sim \chi_2^2(2\gamma)$ which is stochastically increasing in the chi-squared non-centrality parameter 2γ (as this represents the power of a chi-squared statistical test against a family of alternatives ordered by γ). Thus $\mathbb{P}_{\gamma_1}[|y| \geq t] > \mathbb{P}_{\gamma_2}[|y| \geq t]$ for any $t > 0$, implying also $\mathbb{P}[x_1 \geq t] = \mathbb{P}_{\gamma_1}[\sqrt{\gamma_1}|y| \geq t] > \mathbb{P}_{\gamma_1}[\sqrt{\gamma_2}|y| \geq t] > \mathbb{P}_{\gamma_2}[\sqrt{\gamma_2}|y| \geq t] = \mathbb{P}[x_2 \geq t]$.

To show claim (2), observe that $\langle u^j \rangle$ is real for any $j \geq 0$, since the law $p(u) \propto e^{x(u+\bar{u})} = e^{2x \cos \theta}$ is conjugation-symmetric. More precisely, $p(u)$ is a von Mises distribution on the circle, for which

$$u_j := \langle u^j \rangle = I_j(2x)/I_0(2x) \quad (77)$$

where $I_j(\cdot)$ is the modified Bessel function of the first kind

$$I_j(2x) = \sum_{m \geq 0} \frac{1}{m!(m+j)!} x^{2m+j}. \quad (78)$$

We have $\partial_x u_j = \langle u^{j+1} + u^{j-1} \rangle - \langle u^j \rangle \langle u + \bar{u} \rangle = u_{j-1} + u_{j+1} - 2u_1 u_j$ and $f(x) = (1 - u_1^2)^2 + (u_2 - u_1^2)^2$, so

$$\begin{aligned} f'(x) &= -4u_1(1 - u_1^2)(1 + u_2 - 2u_1^2) + 2(u_2 - u_1^2)[(u_1 + u_3 - 2u_1 u_2) - 2u_1(1 + u_2 - 2u_1^2)] \\ &= -4u_1(1 + u_2 - 2u_1^2)^2 + 2(u_2 - u_1^2)(u_1 + u_3 - 2u_1 u_2). \end{aligned}$$

We then make the following observations:

- It is clear from definition that $I_j(2x) > 0$ for any $x > 0$ and $j \geq 0$, hence $u_1 = I_1(2x)/I_0(2x) > 0$.
- We have $u_2 - u_1^2 = I_0(2x)^{-2}(I_2(2x)I_0(2x) - I_1(2x)^2)$, where $I_0(2x)^{-2} > 0$ and

$$\begin{aligned} I_2(2x)I_0(2x) - I_1(2x)^2 &= \sum_{p,q \geq 0} \frac{1}{p!(p+2)!} x^{2p+2} \frac{1}{q!q!} x^{2q} - \sum_{p,q \geq 0} \frac{1}{p!(p+1)!} x^{2p+1} \frac{1}{q!(q+1)!} x^{2q+1} \\ &= \sum_{k \geq 0} x^{2k+2} \sum_{p,q: p+q=k} \frac{1}{p!(p+2)!q!q!} - \frac{1}{p!(p+1)!q!(q+1)!} \\ &= \sum_{k \geq 0} x^{2k+2} \sum_{p,q: p+q=k} \frac{1}{k!(k+2)!} \binom{k}{p} \binom{k+2}{q} - \frac{1}{(k+1)!(k+1)!} \binom{k+1}{p} \binom{k+1}{q} \\ &= \sum_{k \geq 0} x^{2k+2} \left(\frac{1}{k!(k+2)!} - \frac{1}{(k+1)!(k+1)!} \right) \binom{2k+2}{k}, \end{aligned}$$

the last equality using Vandermonde's identity. Here $\frac{1}{k!(k+2)!} - \frac{1}{(k+1)!(k+1)!} < 0$ for every $k \geq 0$, so $u_2 - u_1^2 < 0$.

- We have similarly $u_1 + u_3 - 2u_1 u_2 = I_0(2x)^{-2}(I_3(2x)I_0(2x) + I_1(2x)I_0(2x) - 2I_2(2x)I_1(2x))$, where

$I_0(2x)^{-2} > 0$ and

$$\begin{aligned}
& I_3(2x)I_0(2x) + I_1(2x)I_0(2x) - 2I_2(2x)I_1(2x) \\
&= \sum_{p,q \geq 0} \frac{1}{p!(p+3)!} x^{2p+3} \frac{1}{q!q!} x^{2q} + \sum_{p,q \geq 0} \frac{1}{p!(p+1)!} x^{2p+1} \frac{1}{q!q!} x^{2q} - 2 \sum_{p,q \geq 0} \frac{1}{p!(p+2)!} x^{2p+2} \frac{1}{q!(q+1)!} x^{2q+1} \\
&= x + \sum_{k \geq 0} x^{2k+3} \left(\sum_{p,q: p+q=k} \frac{1}{p!(p+3)!q!q!} + \sum_{p,q: p+q=k+1} \frac{1}{p!(p+1)!q!q!} - 2 \sum_{p,q: p+q=k} \frac{1}{p!(p+2)!q!(q+1)!} \right) \\
&= x + \sum_{k \geq 0} x^{2k+3} \left(\sum_{p,q: p+q=k} \frac{1}{k!(k+3)!} \binom{k}{p} \binom{k+3}{q} + \sum_{p,q: p+q=k+1} \frac{1}{(k+1)!(k+2)!} \binom{k+1}{p} \binom{k+2}{q} \right. \\
&\quad \left. - 2 \sum_{p,q: p+q=k} \frac{1}{(k+1)!(k+2)!} \binom{k+1}{p} \binom{k+2}{q} \right) \\
&= x + \sum_{k \geq 0} x^{2k+3} \left(\frac{1}{k!(k+3)!} \binom{2k+3}{k} + \frac{1}{(k+1)!(k+2)!} \binom{2k+3}{k+1} - \frac{2}{(k+1)!(k+2)!} \binom{2k+3}{k} \right) \\
&= x + \sum_{k \geq 0} x^{2k+3} \frac{1}{(k+1)!(k+2)!} \binom{2k+3}{k} \left(\frac{k+1}{k+3} + \frac{k+3}{k+1} - 2 \right).
\end{aligned}$$

This summand is positive for every $k \geq 0$, hence $u_1 + u_3 - 2u_1u_2 > 0$.

Combining the above yields $f'(x) < 0$ as desired, which concludes the proof. \square

Proof of Theorem 3.10. The fixed-point equation (41) is $q = F(\lambda q)$, for the function $F(\gamma)$ of Lemma B.1. Here $q = 0$ is a fixed point because $F(0) = 0$. Since $q \mapsto F(\lambda q)$ is bounded, increasing, and strictly concave, this is the only fixed point when $1 \geq \partial_q F(\lambda q)|_{q=0} = \lambda$, and there exists a unique other positive fixed point $q_* > 0$ when $1 < \partial_q F(\lambda q)|_{q=0} = \lambda$. Furthermore, $\partial_q \Psi_{\text{gs}}(qI) = -\lambda q + \lambda - \frac{\lambda}{2} \text{mmse}(\lambda q) = \lambda[F(\lambda q) - q]$. When $\lambda \in (0, 1]$, we have $q > F(\lambda q)$ for all $q > 0$, so $\Psi_{\text{gs}}(qI)$ attains its unique maximum at $q = 0$. When $\lambda > 1$, we have $q < F(\lambda q)$ for $q < q_*$ and $q > F(\lambda q)$ for $q > q_*$, so $\Psi_{\text{gs}}(qI)$ attains its unique maximum at $q = q_*$.

Proposition 3.9 then implies that (42) holds, and that $\mathbf{q} = \mathbf{0}$ and $\mathbf{q} = q_*I$ are, respectively, the unique global maximizer of Ψ_{gs} in the two cases $\lambda \in (0, 1]$ and $\lambda > 1$. The remaining statements on $I(G_*, Y)$, MMSE, and overlap concentration then follow from Theorem 3.1. \square

Example of non-identity critical point for $\mathbb{S}\mathbb{O}(k)$ -synchronization.

Proposition B.2. Consider the single-channel $\mathbb{S}\mathbb{O}(k)$ -synchronization model of Example 3.5, with $k \geq 3$. If $\lambda > \lambda_c := k$, then there exists a scalar value $q_* > 0$ for which $\nabla \Psi_{\text{gs}}(\text{diag}(q_*, 0, \dots, 0)) = 0$.

Proof. Write $F(\mathbf{q}) = \mathbb{E}_{\mathbf{g}_*, \mathbf{z}} \langle \mathbf{g} \rangle_{\mathbf{q}}^\top \langle \mathbf{g} \rangle_{\mathbf{q}}$, so $\nabla \Psi_{\text{gs}}(\mathbf{q}) = 0$ if and only if $\mathbf{q} = F(\mathbf{q})$.

We claim that for any \mathbf{q} of the form $\mathbf{q} = \text{diag}(q, 0, \dots, 0)$, we have $F(\mathbf{q}) = \text{diag}(q', 0, \dots, 0)$ for some other $q' \geq 0$. To see this, momentarily let $\mathbf{g}_1 \in \mathbb{R}^k$ and $\mathbf{g}_{2:k} \in \mathbb{R}^{k \times (k-1)}$ denote the first and remaining $k-1$ columns of \mathbf{g} . Observe that when $\mathbf{q} = \text{diag}(q, 0, \dots, 0)$, \mathbf{y} is independent of $\mathbf{g}_{2:k}$ given \mathbf{g}_1 . Hence, for any fixed $\mathbf{h} \in \mathbb{S}\mathbb{O}(k-1)$, we have $\mathbb{E}[\mathbf{g}_{2:k} \mathbf{h} | \mathbf{y}] = \mathbb{E}[\mathbb{E}[\mathbf{g}_{2:k} \mathbf{h} | \mathbf{g}_1, \mathbf{y}] | \mathbf{y}] = \mathbb{E}[\mathbb{E}[\mathbf{g}_{2:k} \mathbf{h} | \mathbf{g}_1] | \mathbf{y}]$. Fixing any \mathbf{g}_1 , we have $\mathbb{E}[\mathbf{g}_{2:k} \mathbf{h} | \mathbf{g}_1] = \mathbb{E}[\mathbf{g}_{2:k} | \mathbf{g}_1]$ by invariance of Haar measure. Thus $\mathbb{E}[\mathbf{g}_{2:k} \mathbf{h} | \mathbf{y}] = \mathbb{E}[\mathbf{g}_{2:k} | \mathbf{y}]$ for every

$\mathbf{h} \in \mathbb{S}\mathbb{O}(k-1)$. Then, taking the average over $\mathbf{h} \sim \text{Haar}(\mathbb{S}\mathbb{O}(k-1))$ which has mean 0 for $k \geq 3$, we get $\langle \mathbf{g}_{2:k} \rangle_{\mathbf{q}} = \mathbb{E}[\mathbf{g}_{2:k} | \mathbf{y}] = 0$, so $F(\mathbf{q})$ is non-zero in only the $(1, 1)$ entry, as claimed.

Thus $\text{diag}(q, 0, \dots, 0)$ is a fixed point if and only if $q = F_{11}(q)$ where $F_{11}(q)$ denotes the $(1, 1)$ -entry of $F(\text{diag}(q, 0, \dots, 0))$. We note that $F_{11}(0) = 0$. By specializing Proposition 3.2(b) to $L = 1$, $\mathbf{q} = \text{diag}(q, 0, \dots, 0)$, and $\mathbf{x} = \mathbf{x}' = \text{diag}(1, 0, \dots, 0)$, we have

$$F'_{11}(q) = \lambda \mathbb{E}_{\mathbf{g}_*, \mathbf{z}} \left[\langle (\mathbf{g}_*^\top \mathbf{g})_{11}^2 \rangle_{\mathbf{q}} - 2(\mathbf{g}_*^\top \langle \mathbf{g} \rangle_{\mathbf{q}})_{11}^2 + \langle \langle \mathbf{g} \rangle_{\mathbf{q}}^\top \langle \mathbf{g} \rangle_{\mathbf{q}} \rangle_{11}^2 \right].$$

When $\mathbf{q} = \mathbf{0}$, we have $\langle \mathbf{g} \rangle_{\mathbf{q}} = 0$ and $\mathbf{g}_*^\top \mathbf{g}$ is equal in law to $\mathbf{g} \sim \text{Haar}(\mathbb{S}\mathbb{O}(k))$, so this gives simply $F'_{11}(0) = \lambda \mathbb{E}_{\mathbf{g}}[(\mathbf{g})_{11}^2] = \frac{\lambda}{k}$. Therefore, if $\lambda > k$, then $F'_{11}(0) > 1$. As $F_{11}(q)$ is continuous and bounded, there must exist a solution $q_* > 0$ to $q = F_{11}(q)$, and hence a fixed point $\text{diag}(q_*, 0, \dots, 0)$ of $\Psi_{\text{gs}}(\mathbf{q})$. \square

C Proofs for quadratic assignment

In this section, we analyze the quadratic assignment model (43). We start by studying the model with linear observations (47) and showing Lemma 4.3 in Section C.1. We then prove Theorem 4.4 in Section C.2, applying the general result of Theorem 2.2 and formalizing an approximation of the free energy by that in a model with the truncated kernel κ^L .

We will use throughout the following elementary observations: Since κ is continuous and \mathcal{X} is compact, there exists a constant $K_0 < \infty$ for which

$$|\kappa(x, y)| < K_0 \text{ for all } x, y \in \mathcal{X}. \quad (79)$$

Furthermore, since $f_\ell(x) = \mu_\ell^{-1} \int \kappa(x, y) f_\ell(y) \rho(dy)$ and $\int |\kappa(x, y) f_\ell(y)| \rho(dy) < K_0 (\int f_\ell(y)^2 \rho(dy))^{1/2} < \infty$, by the dominated convergence theorem $\lim_{x' \rightarrow x} f_\ell(x') = f_\ell(x)$. Thus each $f_\ell(x)$ is also continuous on \mathcal{X} , so there exist constants $C_\ell < \infty$ for which

$$|f_\ell(x)| < C_\ell \text{ for all } x \in \mathcal{X} \text{ and } \ell \geq 1. \quad (80)$$

C.1 Mutual information of the linear model

Proof of Lemma 4.3. We apply the result of [GR09] for Bayesian estimation in compound decision models. Fixing $\{x_i\}_{i=1}^N$, let us compare the two observation models

$$\mathbf{y}_i = \sqrt{\lambda} \mathbf{q}^{1/2} \mathbf{u}(x_{\pi_*(i)}) + \mathbf{z}_i \text{ for } i = 1, \dots, N \quad (81)$$

$$\mathbf{y}'_i = \sqrt{\lambda} \mathbf{q}^{1/2} \mathbf{v}_{*i} + \mathbf{z}'_i \text{ for } i = 1, \dots, N \quad (82)$$

where $\{\mathbf{v}_{*i}\}_{i=1}^N$ are drawn i.i.d. (with replacement) from the empirical distribution of $\{\mathbf{u}(x_i)\}_{i=1}^N$, and $\mathbf{z}_i, \mathbf{z}'_i \stackrel{iid}{\sim} \mathcal{N}(0, I)$. Let $i_\lambda(\pi_*, Y_{\text{lin}})$ be the mutual information between π_* and $Y_{\text{lin}} = (\mathbf{y}_i)_{i=1}^N$ in the model (81), and let $i_\lambda(V_*, Y'_{\text{lin}})$ be the mutual information between $V_* = (\mathbf{v}_{*i})_{i=1}^N$ and $Y'_{\text{lin}} = (\mathbf{y}'_i)_{i=1}^N$ in the model (82). In (82), the samples $(\mathbf{v}_{*i}, \mathbf{y}'_i)$ are i.i.d. given $\{x_i\}_{i=1}^N$, and a direct calculation gives

$$\frac{1}{N} i_\lambda(V_*, Y'_{\text{lin}}) = \mathbb{E}_{\mathbf{v}_*, \mathbf{z}'} \left[\frac{\lambda}{2} \mathbf{v}_*^\top \mathbf{q} \mathbf{v}_* - \log \mathbb{E}_{\mathbf{v}} \exp \left(-\frac{\lambda}{2} \mathbf{v}^\top \mathbf{q} \mathbf{v} + \lambda \mathbf{v}^\top \mathbf{q} \mathbf{v}_* + \sqrt{\lambda} \mathbf{v}^\top \mathbf{q}^{1/2} \mathbf{z}' \right) \right]$$

where $\mathbb{E}_{\mathbf{v}}, \mathbb{E}_{\mathbf{v}_*}$ are expectations over $\mathbf{v}, \mathbf{v}_* \in \mathbb{R}^L$ sampled uniformly at random from the empirical distribution of $\{\mathbf{u}(x_i)\}_{i=1}^N$.

By the i-mmse relation [GSV05], we have

$$\begin{aligned}\frac{\partial}{\partial \lambda} i_\lambda(\pi_*, Y_{\text{lin}}) &= \frac{1}{2} \sum_{i=1}^N \mathbb{E} \left\| \mathbf{q}^{1/2} \mathbf{u}(x_{\pi_*(i)}) - \mathbf{q}^{1/2} \mathbb{E}[\mathbf{u}(x_{\pi(i)}) \mid Y_{\text{lin}}] \right\|_2^2 =: \frac{1}{2} \text{mmse}_{\pi_*}(\lambda), \\ \frac{\partial}{\partial \lambda} i_\lambda(V_*, Y'_{\text{lin}}) &= \frac{1}{2} \sum_{i=1}^N \mathbb{E} \left\| \mathbf{q}^{1/2} \mathbf{v}_{*i} - \mathbf{q}^{1/2} \mathbb{E}[\mathbf{v}_i \mid Y'_{\text{lin}}] \right\|_2^2 =: \frac{1}{2} \text{mmse}_{V_*}(\lambda).\end{aligned}$$

The analyses of [GR09, Theorem 5.1, Corollary 5.2] extend verbatim to a multivariate setting, to show $|\text{mmse}_{\pi_*}(\lambda) - \text{mmse}_{V_*}(\lambda)| \leq C_\lambda$ for a constant C_λ depending only on $\max_{i=1}^N \|\sqrt{\lambda} \mathbf{u}(x_i) \mathbf{q}^{1/2}\|_2$. Then, applying $i_0(\pi_*, Y_{\text{lin}}) = i_0(V_*, Y'_{\text{lin}}) = 0$ and integrating over $\lambda \in [0, 1]$, we obtain

$$\left| \frac{1}{N} i_1(\pi_*, Y_{\text{lin}}) - \frac{1}{N} i_1(V_*, Y'_{\text{lin}}) \right| \leq \frac{C}{N}$$

for some constant $C > 0$ depending on $(C_\ell)_{\ell \leq L}$ from (80).

Here, $i_1(\pi_*, Y_{\text{lin}}) = i(\pi_*, Y_{\text{lin}})$ is the mutual information of interest in the model (47). Since the empirical law of $\{x_i\}_{i=1}^N$ converges weakly to ρ , by continuity of $\mathbf{u}(x)$ we have that the law of \mathbf{v}, \mathbf{v}_* (i.e. the empirical law of $\{\mathbf{u}(x_i)\}_{i=1}^N$) converges weakly to the law of $\mathbf{u}(x)$ when $x \sim \rho$. Then by the dominated convergence theorem, $\lim_{N \rightarrow \infty} \frac{1}{N} i_1(V_*, Y'_{\text{lin}}) = i(x, \mathbf{y})$ as defined in the lemma. \square

C.2 Mutual information of the quadratic model

We now bound the discrepancy in mutual information due to truncation of the kernel.

Lemma C.1. *Suppose Assumption 4.1 holds, and let K_0 satisfy (79). Let $I(\pi_*, Y)$ be the signal-observation mutual information in the model (43), and let $I(\pi_*, Y^L)$ be that in the analogous model with kernel κ^L defined by (44). Then for any $\epsilon > 0$, there exists $L_0 = L_0(\epsilon)$ such that for all $L \geq L_0$ and $N \geq 1$,*

$$\frac{1}{N} |I(\pi_*, Y) - I(\pi_*, Y^L)| \leq K_0 \epsilon.$$

Proof. By the uniform convergence of κ^L to κ given by Mercer's theorem (Theorem 4.2), for any $\epsilon > 0$, there exists an $L_0 = L_0(\epsilon)$ such that for all $L \geq L_0$,

$$\sup_{x, y} |\kappa^L(x, y) - \kappa(x, y)| < \epsilon. \quad (83)$$

From here on, fix any $L \geq L_0$. Write as shorthand

$$\kappa_{ij} = \kappa(x_{\pi(i)}, x_{\pi(j)}), \quad \kappa_{*ij} = \kappa(x_{\pi_*(i)}, x_{\pi_*(j)}), \quad \kappa_{ij}^L = \kappa^L(x_{\pi(i)}, x_{\pi(j)}), \quad \kappa_{*ij}^L = \kappa^L(x_{\pi_*(i)}, x_{\pi_*(j)}).$$

The Hamiltonians associated to the model (43) and the one defined by κ^L in place of κ are, respectively,

$$H(\pi; \pi_*, Z) := -\frac{1}{2N} \sum_{i < j} \kappa_{ij}^2 + \frac{1}{N} \sum_{i < j} \kappa_{*ij} \kappa_{ij} + \frac{1}{\sqrt{N}} \sum_{i < j} \kappa_{ij} z_{ij}, \quad (84)$$

$$H^L(\pi; \pi_*, Z) := -\frac{1}{2N} \sum_{i < j} (\kappa_{ij}^L)^2 + \frac{1}{N} \sum_{i < j} \kappa_{*ij}^L \kappa_{ij}^L + \frac{1}{\sqrt{N}} \sum_{i < j} \kappa_{ij}^L z_{ij}. \quad (85)$$

Let \mathcal{F}_N^∞ and \mathcal{F}_N^L denote the free energies associated with these Hamiltonians,

$$\mathcal{F}_N^\infty := \frac{1}{N} \mathbb{E}_{\pi_*, Z} \log \mathbb{E}_\pi \exp H(\pi; \pi_*, Z) \quad \text{and} \quad \mathcal{F}_N^L := \frac{1}{N} \mathbb{E}_{\pi_*, Z} \log \mathbb{E}_\pi \exp H^L(\pi; \pi_*, Z). \quad (86)$$

Then by the same calculations as (68),

$$\frac{1}{N} I(\pi_*, Y) = \frac{1}{2N^2} \mathbb{E}_{\pi_*} \sum_{i < j} \kappa_{*ij}^2 - \mathcal{F}_N^\infty, \quad \frac{1}{N} I(\pi_*, Y^L) = \frac{1}{2N^2} \mathbb{E}_{\pi_*} \sum_{i < j} (\kappa_{*ij}^L)^2 - \mathcal{F}_N^L.$$

Thus, with H and H^L defined in (84) and (85), we have

$$\frac{1}{N} |I(\pi_*, Y) - I(\pi_*, Y^L)| \leq \frac{1}{2N^2} \mathbb{E}_{\pi_*} \sum_{i < j} |\kappa_{*ij}^2 - (\kappa_{*ij}^L)^2| + \frac{1}{N} \mathbb{E}_{\pi_*, Z} \sup_{\pi \in \mathbb{S}_N} |H(\pi; \pi_*, Z) - H^L(\pi; \pi_*, Z)|. \quad (87)$$

By the boundedness of the kernels (79), and (83), for any π, π_* we have

$$|\kappa_{ij}^2 - (\kappa_{ij}^L)^2|, |\kappa_{*ij} \kappa_{ij} - \kappa_{*ij}^L \kappa_{ij}^L|, |\kappa_{*ij}^2 - (\kappa_{*ij}^L)^2| \leq 2K_0 \epsilon.$$

Set $z_{ii} = 0$ and $\kappa_{ii} = \kappa(x_{\pi(i)}, x_{\pi(i)})$ for all $i = 1, \dots, N$, set $\kappa_{ij} = \kappa_{ji}$, $\kappa_{ij}^L = \kappa_{ji}^L$, $z_{ij} = z_{ji}$ for all $i > j$, and define the symmetric matrices $K = (\kappa_{ij})_{i,j=1}^N$, $K^L = (\kappa_{ij}^L)_{i,j=1}^N$, and $Z = (z_{ij})_{i,j=1}^N$. Then, applying the von-Neumann trace inequality,

$$\left| \sum_{i < j} \kappa_{ij} z_{ij} - \kappa_{ij}^L z_{ij} \right| = \frac{1}{2} |\text{Tr} Z(K - K^L)| \leq \frac{1}{2} \|Z\|_{\text{op}} \|K - K^L\|_* = \frac{1}{2} \|Z\|_{\text{op}} \text{Tr}(K - K^L)$$

where $\|\cdot\|_*$ denotes the nuclear norm, and the last equality follows because $\kappa - \kappa^L$ remains a positive-semidefinite kernel, so $K - K^L$ is a positive-semidefinite matrix. Applying $\text{Tr}(K - K^L) \leq K_0 N \epsilon$ by (83) and combining the above into (87), we obtain

$$\frac{1}{N} |I(\pi_*, Y) - I(\pi_*, Y^L)| \leq 2K_0 \epsilon + \frac{K_0 \epsilon}{2\sqrt{N}} \mathbb{E} \|Z\|_{\text{op}}.$$

Denote by \tilde{Z} a copy of Z with diagonal entries replaced by independent $\mathcal{N}(0, 2)$ variables, and observe that $\mathbb{E}[(u^\top Z u - v^\top Z v)^2] \leq \mathbb{E}[(u^\top \tilde{Z} u - v^\top \tilde{Z} v)^2]$ for any unit vectors $u, v \in \mathbb{R}^N$. Then by a standard application of the Sudakov-Fernique inequality (see e.g. [Ver18, Exercise 7.3.5]), $\mathbb{E} \|Z\|_{\text{op}} \leq \mathbb{E} \|\tilde{Z}\|_{\text{op}} \leq 2\sqrt{N}$, and the result follows upon adjusting the value of ϵ . \square

We are now ready to prove Theorem 4.4.

Proof of Theorem 4.4. We apply Theorem 2.2. Fixing any $L \geq 1$, define $\mathcal{G}_N = \mathbb{S}_N$, the feature map $\phi : \mathbb{S}_N \rightarrow (\mathbb{R}^L)^N$ by (45), and the bilinear forms \bullet, \otimes and inclusion map $\iota(\cdot)$ by (46). It is then direct to check that all conditions of Assumption 2.1 hold. The quantities $K(\mathcal{G}_N)$, $D(\mathcal{G}_N)$, and $L(\epsilon; \mathcal{G}_N)$ for any fixed $\epsilon > 0$ in Theorem 2.2 are bounded by a constant due to (79), and as $N \rightarrow \infty$,

$$\begin{aligned} \|Q(\text{Id}, \text{Id})\|_{\mathcal{L}}^2 &= \left\| \frac{1}{N} \sum_{i=1}^N \mathbf{u}(x_i) \mathbf{u}(x_i)^\top \right\|_F^2 \rightarrow \|\mathbb{E}_{x \sim \rho} \mathbf{u}(x) \mathbf{u}(x)^\top\|_F^2 = \mathbb{E}_{x, x' \stackrel{iid}{\sim} \rho} (\mathbf{u}(x)^\top \mathbf{u}(x'))^2 = \mathbb{E}_{x, x' \stackrel{iid}{\sim} \rho} [\kappa^L(x, x')^2], \\ \langle \mathbf{q}, Q(\text{Id}, \text{Id}) \rangle_{\mathcal{L}} &= \text{Tr} \mathbf{q} \left(\frac{1}{N} \sum_{i=1}^N \mathbf{u}(x_i) \mathbf{u}(x_i)^\top \right) \rightarrow \mathbb{E}_{x_* \sim \rho} \text{Tr} \mathbf{q} \mathbf{u}(x_*) \mathbf{u}(x_*)^\top = \mathbb{E}_{x_* \sim \rho} \mathbf{u}(x_*)^\top \mathbf{q} \mathbf{u}(x_*) \end{aligned}$$

under Assumption 4.1. Hence from Theorem 2.2, Lemma 4.3, and the forms (15) and (16) for the mutual informations, we have

$$\lim_{N \rightarrow \infty} \frac{1}{N} I(\pi_*, Y^L) = \frac{1}{4} \mathbb{E}_{x, x' \stackrel{iid}{\sim} \rho} [\kappa^L(x, x')^2] - \sup_{\mathbf{q} \in \text{Sym}_{\geq 0}^{L \times L}} \Psi_{\text{qa}}^L(\mathbf{q}). \quad (88)$$

Here, $\sup_{\mathbf{q} \in \text{Sym}_{\geq 0}^{L \times L}} \Psi_{\text{qa}}^L(\mathbf{q})$ is non-decreasing in L , as a restriction of this supremum to $\mathbf{q} \in \text{Sym}_{\geq 0}^{L \times L}$ having last row and column equal to 0 gives the optimization for dimension $L - 1$. Thus the limit Ψ_∞ exists in $(-\infty, \infty]$, and

$$\lim_{L \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{N} I(\pi_*, Y^L) = \frac{1}{4} \mathbb{E}_{x, x' \stackrel{iid}{\sim} \rho} [\kappa(x, x')^2] - \Psi_\infty.$$

Finally, Lemma C.1 shows that $N^{-1}I(\pi_*, Y^L)$ converges to $N^{-1}I(\pi_*, Y)$ as $L \rightarrow \infty$, uniformly over all $N \geq 1$. Thus the limits in L and N on the left side may be interchanged. Since $I(\pi_*, Y)$ is bounded below by 0 and $\mathbb{E}[\kappa(x, x')^2]$ is bounded above due to (79), this implies that Ψ_∞ is finite, concluding the proof. \square

D Group representations

We give a brief review of relevant notions from the representation theory of compact groups, and refer readers to [BTD13, Chapter 2] and [Kna01, Chapter 1] for further background.

Throughout, \mathcal{G} is a compact group, and representations are always finite-dimensional and continuous. We will choose to fix the bases and inner-product structures for \mathbb{C}^k and \mathbb{R}^k , thus identifying representations as $k \times k$ matrices.

D.1 Complex representations

A (complex) representation of \mathcal{G} is a continuous map $\phi : \mathcal{G} \rightarrow \mathbb{C}^{k \times k}$ satisfying the group homomorphism properties $\phi(gh) = \phi(g)\phi(h)$, $\phi(g^{-1}) = \phi(g)^{-1}$, and $\phi(\text{Id}) = I_{k \times k}$. The representation is *trivial* if $\phi(g) = I_{k \times k}$ for all $g \in \mathcal{G}$, and *non-trivial* otherwise.

Definition D.1. Given a representation $\phi : \mathcal{G} \rightarrow \mathbb{C}^{k \times k}$, a complex linear subspace $W \subseteq \mathbb{C}^k$ is invariant if $\phi(g)w \in W$ for every $g \in \mathcal{G}$ and $w \in W$. The representation ϕ is \mathbb{C} -*irreducible* if there are no complex invariant subspaces other than $W = \{0\}$ and $W = \mathbb{C}^k$.

Definition D.2. Given two representations $\phi : \mathcal{G} \rightarrow \mathbb{C}^{k \times k}$ and $\phi' : \mathcal{G} \rightarrow \mathbb{C}^{k' \times k'}$, a map $U \in \mathbb{C}^{k' \times k}$ is an *intertwining map* of ϕ with ϕ' if $U\phi(g) = \phi'(g)U$ for all $g \in \mathcal{G}$. It is an *isomorphism* if $k = k'$ and U is invertible. The representations ϕ, ϕ' are *isomorphic* (denoted $\phi \cong \phi'$) if there exists such an isomorphism, i.e. an invertible map $U \in \mathbb{C}^{k \times k}$ such that $\phi(g) = U^{-1}\phi'(g)U$ for all $g \in \mathcal{G}$; otherwise ϕ and ϕ' are *distinct*.

Theorem D.3 (Schur's Lemma, [BTD13] Theorem 2.1.10). *Let $\phi : \mathcal{G} \rightarrow \mathbb{C}^{k \times k}$ and $\phi' : \mathcal{G} \rightarrow \mathbb{C}^{k' \times k'}$ be two \mathbb{C} -irreducible representations of \mathcal{G} .*

- (a) *If $U \in \mathbb{C}^{k' \times k}$ is an intertwining map of ϕ with ϕ' , then either $U = 0$ or U is an isomorphism.*
- (b) *If $U \in \mathbb{C}^{k \times k}$ is an intertwining map of ϕ with itself, then $U = \lambda I_{k \times k}$ for some $\lambda \in \mathbb{C}$.*

An intertwining map U of ϕ with itself is a map that commutes with $\phi(g)$ for all $g \in \mathcal{G}$; part (b) states that when ϕ is \mathbb{C} -irreducible, any such map is a multiple of the identity. If \mathcal{G} is abelian, then $U = \phi(g_0)$ is such an intertwining map for any $g_0 \in \mathcal{G}$, so an immediate consequence is the following.

Corollary D.4 ([[BTD13](#)] Proposition 2.1.13). *If \mathcal{G} is abelian and $\phi : \mathcal{G} \rightarrow \mathbb{C}^{k \times k}$ is \mathbb{C} -irreducible, then $k = 1$.*

A representation $\phi : \mathcal{G} \rightarrow \mathbb{C}^{k \times k}$ is *unitary* if $\phi(g)$ is a unitary matrix for all $g \in \mathcal{G}$, i.e. $\phi(g)^* \phi(g) = I_{k \times k}$. For compact \mathcal{G} , any representation is isomorphic to a unitary representation [[BTD13](#), Theorem 2.1.7].

Theorem D.5 (Complete reducibility, [[Kna01](#)] Theorem 1.12(d)). *Let $\phi : \mathcal{G} \rightarrow \mathbb{C}^{k \times k}$ be a unitary representation of a compact group \mathcal{G} . Then there exists a unitary map $U \in \mathbb{C}^{k \times k}$ and \mathbb{C} -irreducible unitary representations $\phi_\ell : \mathcal{G} \rightarrow \mathbb{C}^{k_\ell \times k_\ell}$ for $\ell = 1, \dots, L$ with $k_1 + \dots + k_L = k$, such that*

$$\phi(g) = U \begin{pmatrix} \phi_1(g) & & \\ & \ddots & \\ & & \phi_L(g) \end{pmatrix} U^{-1}. \quad (89)$$

If a representation $\phi : \mathcal{G} \rightarrow \mathbb{C}^{k \times k}$ admits a decomposition of the form (89) for some invertible map $U \in \mathbb{C}^{k \times k}$ (where ϕ, U and ϕ_1, \dots, ϕ_L are not necessarily unitary), then we say that ϕ_1, \dots, ϕ_L are *subrepresentations* contained in ϕ , and ϕ is a *direct sum* of ϕ_1, \dots, ϕ_L , denoted $\phi \cong \phi_1 \oplus \dots \oplus \phi_L$.

Definition D.6. The *character* $\chi_\phi : \mathcal{G} \rightarrow \mathbb{C}$ of a representation $\phi : \mathcal{G} \rightarrow \mathbb{C}^{k \times k}$ is the function

$$\chi_\phi(g) = \text{Tr } \phi(g).$$

Theorem D.7 (Schur orthogonality, [[Kna01](#)] Theorem 1.12(b), [[BTD13](#)] Theorem 2.4.11). *Let \mathcal{G} be a compact group, and let $\phi_\ell : \mathcal{G} \rightarrow \mathbb{C}^{k_\ell \times k_\ell}$ be any distinct, \mathbb{C} -irreducible, and unitary representations of \mathcal{G} , with corresponding characters $\chi_\ell : \mathcal{G} \rightarrow \mathbb{C}$.*

(a) *The normalized matrix entry functions*

$$\{k_\ell^{1/2} \phi_\ell(\cdot)_{ij}\}_{\ell=1, \dots, L, 1 \leq i, j \leq k_\ell}$$

are orthonormal in the complex inner-product space $L^2(\mathcal{G})$ with respect to Haar measure on \mathcal{G} .

(b) *The characters $\{\chi_\ell : \ell = 1, \dots, L\}$ are also orthonormal in $L^2(\mathcal{G})$.*

We remark that if $\phi \cong \phi'$ and $\phi \cong \phi_1 \oplus \dots \oplus \phi_L$, then by definition, their characters satisfy $\chi_\phi = \chi_{\phi'}$ and $\chi_\phi = \chi_{\phi_1} + \dots + \chi_{\phi_L}$. An immediate consequence of this and Theorem D.7(b) is the following.

Corollary D.8 ([[BTD13](#)] Theorem 2.4.12). *Two representations ϕ, ϕ' of \mathcal{G} are isomorphic if and only if $\chi_\phi = \chi_{\phi'}$, i.e. $\chi_\phi(g) = \chi_{\phi'}(g)$ for all $g \in \mathcal{G}$.*

We conclude with a basic proposition showing that if two unitary representations are isomorphic, then the isomorphism between these representations may also be taken to be a unitary transform.

Proposition D.9. *Let $\phi, \phi' : \mathcal{G} \rightarrow \mathbb{C}^{k \times k}$ be isomorphic unitary representations. Then there exists a unitary matrix $U \in \mathbb{C}^{k \times k}$ for which $\phi'(g) = U\phi(g)U^*$ for all $g \in \mathcal{G}$.*

Proof. Applying Theorem D.5, we may write $\phi(g)$ in the form (89) for some unitary matrix $U \in \mathbb{C}^{k \times k}$ and unitary \mathbb{C} -irreducible sub-representations ϕ_1, \dots, ϕ_L , and similarly for ϕ' and some $U', \phi'_1, \dots, \phi'_M$. Since $\chi_{\phi_1} + \dots + \chi_{\phi_L} = \chi_{\phi'_1} + \dots + \chi_{\phi'_M}$ and characters of distinct irreducible representations are distinct orthogonal functions in $L^2(\mathcal{G})$, this implies that $L = M$ and $\phi_1 \cong \phi'_1, \dots, \phi_L \cong \phi'_L$ under some ordering of these irreducible sub-representations. Absorbing this ordering as a permutation into U and U' , it suffices to prove the proposition in the case where ϕ, ϕ' are isomorphic and \mathbb{C} -irreducible.

Since ϕ, ϕ' are isomorphic, there exists an invertible matrix $U \in \mathbb{C}^{k \times k}$ for which $\phi(g) = U^{-1}\phi'(g)U$ for all $g \in \mathcal{G}$; we must show that we may take U to be unitary. Since $\phi(g)$ is unitary, we have $I = \phi(g)\phi(g)^* = U^{-1}\phi'(g)UU^*\phi'(g)^*U^{-*}$. Then, since $\phi'(g)$ is unitary, rearranging this gives $UU^*\phi'(g) = \phi'(g)UU^*$. Thus UU^* is an intertwining map of ϕ' with itself. Since ϕ' is irreducible, Schur's lemma implies $UU^* = \alpha I$ for some $\alpha \in \mathbb{C}$. We must have $\alpha \in \mathbb{R}$ and $\alpha > 0$ because UU^* is Hermitian positive-definite. Thus $\tilde{U} = U/\sqrt{\alpha}$ is unitary and $\phi(g) = \tilde{U}^*\phi'(g)U$ as claimed. \square

D.2 Real representations

A representation ϕ of \mathcal{G} is a *real representation* if $\phi(g)$ is real-valued for all $g \in \mathcal{G}$, i.e. ϕ is a map $\phi : \mathcal{G} \rightarrow \mathbb{R}^{k \times k}$. It is *orthogonal* if furthermore $\phi(g)$ is an orthogonal matrix for all $g \in \mathcal{G}$, i.e. $\phi(g)^\top \phi(g) = I_{k \times k}$.

Definition D.10. Given a real representation $\phi : \mathcal{G} \rightarrow \mathbb{R}^{k \times k}$, a real linear subspace $W \subseteq \mathbb{R}^k$ is invariant if $\phi(g)w \in W$ for every $g \in \mathcal{G}$ and $w \in W$. The representation is *real-irreducible* (or *\mathbb{R} -irreducible*) if it has no real invariant subspaces other than $W = \{0\}$ and $W = \mathbb{R}^k$.

The following statements are analogues of Schur's lemma and complete reducibility in the real setting. We include their proofs for completeness, which are similar to their complex counterparts.

Theorem D.11. Let $\phi : \mathcal{G} \rightarrow \mathbb{R}^{k \times k}$ and $\phi' : \mathcal{G} \rightarrow \mathbb{R}^{k' \times k'}$ be two real-irreducible representations of \mathcal{G} .

- (a) If $U \in \mathbb{R}^{k' \times k}$ is an intertwining map of ϕ with ϕ' , then either $U = 0$ or U is an isomorphism.
- (b) If $U \in \mathbb{R}^{k \times k}$ is an intertwining map of ϕ with itself, and U has at least one real eigenvalue, then $U = \lambda I_{k \times k}$ for some $\lambda \in \mathbb{R}$.

Proof. For (a), since $U\phi = \phi'U$, we have that $\ker U \subseteq \mathbb{R}^k$ is a real invariant subspace of ϕ , and $\text{im } U \subseteq \mathbb{R}^{k'}$ is a real invariant subspace of ϕ' . Thus either $\ker U = \mathbb{R}^k$ in which case $U = 0$, or $\ker U = 0$ and $\text{im } U = \mathbb{R}^{k'}$ in which case $k = k'$ and U is an isomorphism.

For part (b), let $\lambda \in \mathbb{R}$ be an eigenvalue of U , and let $V_\lambda = \ker(U - \lambda I) \subseteq \mathbb{R}^k$ be its corresponding eigenspace. For any $v \in V_\lambda$ and $g \in \mathcal{G}$, we have $U\phi(g)v = \phi(g)Uv = \lambda\phi(g)v$, so $\phi(g)v \in V_\lambda$. Thus V_λ is a real invariant subspace. We have $V_\lambda \neq \{0\}$ since λ is an eigenvalue, so $V_\lambda = \mathbb{R}^k$ and $U = \lambda I_{k \times k}$. \square

Theorem D.12. Let $\phi : \mathcal{G} \rightarrow \mathbb{R}^{k \times k}$ be an orthogonal representation of a compact group \mathcal{G} . Then it is an orthogonal direct sum of real-irreducible components, i.e., there exists an orthogonal map $U \in \mathbb{R}^{k \times k}$ and real-irreducible orthogonal representations $\phi_\ell : \mathcal{G} \rightarrow \mathbb{R}^{k_\ell \times k_\ell}$ for $\ell = 1, \dots, L$ with $k_1 + \dots + k_L = k$, such that

$$\phi(g) = U \begin{pmatrix} \phi_1(g) & & \\ & \ddots & \\ & & \phi_L(g) \end{pmatrix} U^\top$$

Proof. If ϕ is real-irreducible, then the statement holds trivially with $L = 1$ and $U = I$. Otherwise, let $W \subset \mathbb{R}^k$ be a real invariant subspace not equal to $\{0\}$ or \mathbb{R}^k , and let W^\perp be its orthogonal complement. For any $v \in W$, $w \in W^\perp$, and $g \in \mathcal{G}$ we have $(\phi(g)w)^\top v = w^\top \phi(g^{-1})v = 0$ because $\phi(g^{-1})v \in W$. So $\phi(g)w \in W^\perp$, implying that W^\perp is also invariant. Thus $\phi(g)$ acts as two separate linear maps on W and W^\perp for all $g \in \mathcal{G}$. Choosing U where the first k_1 columns and last $k_2 = k - k_1$ columns form orthonormal bases for W and W^\perp , respectively, this implies that each $\phi(g)$ takes the form

$$\phi(g) = U \begin{pmatrix} \phi_1(g) & \\ & \phi_2(g) \end{pmatrix} U^\top \quad \Leftrightarrow \quad \begin{pmatrix} \phi_1(g) & \\ & \phi_2(g) \end{pmatrix} = U^\top \phi(g) U \quad (90)$$

for some functions $\phi_1 : \mathcal{G} \rightarrow \mathbb{R}^{k_1 \times k_1}$ and $\phi_2 : \mathcal{G} \rightarrow \mathbb{R}^{k_2 \times k_2}$. Continuity, orthogonality, and the group representation properties of ϕ_1, ϕ_2 follow from the equality on the right side of (90) and the corresponding properties for ϕ . Thus ϕ_1, ϕ_2 are real orthogonal sub-representations of \mathcal{G} , of lower dimensionalities $k_1, k_2 < k$, and the result follows from induction on k . \square

Any real representation $\phi : \mathcal{G} \rightarrow \mathbb{R}^{k \times k}$ that is \mathbb{C} -irreducible (when viewed as a complex representation under the embedding $\mathbb{R}^{k \times k} \subset \mathbb{C}^{k \times k}$) is, by definition, also real-irreducible. However the converse is not true, and real-irreducible representations may be reducible in the complex sense. An example is the standard representation of $\mathcal{G} = \mathbb{S}\mathbb{O}(2)$ in (35), which has no real invariant subspaces, but two orthogonal complex invariant subspaces spanned by $(1, i)$ and $(i, 1)$. This example shows also that the extra assumption in Theorem D.11(b) of U having a real eigenvalue cannot, in general, be removed: $\mathcal{G} = \mathbb{S}\mathbb{O}(2)$ is abelian, so any $U \in \mathbb{S}\mathbb{O}(2)$ is an intertwining map of $\mathbb{S}\mathbb{O}(2)$ with itself, but U may not be a multiple of the identity.

Theorem D.13 (Classification of real-irreducible representations, [BTD13] Table 2.6.2, Theorem 2.6.3). *Let $\phi : \mathcal{G} \rightarrow \mathbb{R}^{k \times k}$ be a real-irreducible representation. Then, as a complex representation in $\mathbb{C}^{k \times k}$, it is either*

- (a) \mathbb{C} -irreducible.
- (b) Isomorphic to the direct sum $\psi \oplus \bar{\psi}$ of two \mathbb{C} -irreducible representations $\psi, \bar{\psi}$ such that $\psi, \bar{\psi}$ are distinct (i.e. $\psi \not\cong \bar{\psi}$), where $\bar{\psi}$ denotes the complex conjugate representation $\bar{\psi}(g) = \overline{\psi(g)}$ for all $g \in \mathcal{G}$.
- (c) Isomorphic to the direct sum $\psi \oplus \psi$ of a \mathbb{C} -irreducible representation ψ with itself, such that $\psi \cong \bar{\psi}$.

We remark that since the sub-representations ψ in case (b) are distinct from those in case (c), the \mathbb{C} -irreducible sub-representations of ϕ must be distinct from those of ϕ' if ϕ, ϕ' are real-irreducible and distinct. This implies also by Theorem D.7 that the corresponding characters $\chi_\phi, \chi_{\phi'}$ are orthogonal (although not necessarily orthonormal) in $L^2(\mathcal{G})$.

Following the terminology of [BTD13, Section 2.6], we call ϕ of “real type”, “complex type”, and “quaternionic type” in these cases (a), (b), and (c) respectively. From the character relations $\chi_\phi = \chi_\psi + \chi_{\bar{\psi}}$ and $\chi_\phi = 2\chi_\psi$ in the latter two cases, and the Schur orthogonality of characters for \mathbb{C} -irreducible representations (Theorem D.7), it is readily deduced that $\rho := \mathbb{E}_{g \sim \text{Haar}(\mathcal{G})}[(\text{Tr } \phi(g))^2]$ takes the value 1, 2, or 4 when ϕ is of real, complex, or quaternionic type respectively, as stated in (34).

A direct consequence of Theorem D.13 and Corollary D.4 is the following.

Corollary D.14. *If \mathcal{G} is abelian and $\phi : \mathcal{G} \rightarrow \mathbb{R}^{k \times k}$ is real-irreducible, then $k = 1$ if ϕ is of real type, and $k = 2$ if ϕ is of complex or quaternionic type.*

Finally, the following is an analogue of Proposition D.9.

Proposition D.15. *Let $\phi, \phi' : \mathcal{G} \rightarrow \mathbb{R}^{k \times k}$ be real representations that are isomorphic. Then there exists a (real) invertible map $U \in \mathbb{R}^{k \times k}$ such that $\phi(g) = U^{-1}\phi'(g)U$ for all $g \in \mathcal{G}$. If furthermore ϕ, ϕ' are orthogonal, then there exists such a map U which is also orthogonal.*

Proof. Since characters of distinct real-irreducible representations are distinct and orthogonal functions of $L^2(\mathcal{G})$, the same argument as in Proposition D.9 shows that $\phi_1 \cong \phi'_1, \dots, \phi_L \cong \phi'_L$ for some ordering of the real-irreducible sub-representations of ϕ, ϕ' , so it suffices to prove the statements when ϕ, ϕ' are isomorphic and real-irreducible.

Since ϕ, ϕ' are isomorphic, there exists an invertible matrix $U \in \mathbb{C}^{k \times k}$ for which $\phi(g) = U^{-1}\phi'(g)U$; we must show that we may take U to be real. Writing the real and imaginary parts $U = P + iQ$, we have $(P + iQ)\phi(g) = \phi'(g)(P + iQ)$. Then $P\phi(g) = \phi'(g)P$ and $Q\phi(g) = \phi'(g)Q$ since ϕ and ϕ' are real, so $(P + \lambda Q)\phi(g) = \phi'(g)(P + \lambda Q)$ for all $\lambda \in \mathbb{R}$. The complex polynomial $f(\lambda) = \det(P + \lambda Q)$ is not identically 0 because it is non-zero at $\lambda = i$. Then there exists also some $\lambda \in \mathbb{R}$ for which $f(\lambda) \neq 0$, implying that $\tilde{U} = P + \lambda Q \in \mathbb{R}^{k \times k}$ is invertible, and $\phi(g) = \tilde{U}^{-1}\phi'(g)\tilde{U}$. This shows the first statement.

Now letting $U \in \mathbb{R}^{k \times k}$ be such that $\phi(g) = U^{-1}\phi'(g)U$, if furthermore ϕ, ϕ' are orthogonal, then the same argument as in Proposition D.9 shows $UU^\top\phi'(g) = \phi'(g)UU^\top$. Here UU^\top is symmetric positive-semidefinite, having all real eigenvalues, so Schur's lemma in the form of Theorem D.11(b) implies $UU^\top = \alpha I$ for some $\alpha > 0$. Thus $\tilde{U} = U/\sqrt{\alpha}$ is orthogonal and $\phi(g) = \tilde{U}^\top\phi'(g)U$, showing the second statement. \square

D.3 Canonical form for the group synchronization model

Consider observations from a model (21) with real orthogonal representations $\phi_\ell : \mathcal{G} \rightarrow \mathbb{R}^{k_\ell \times k_\ell}$. By Theorem D.12 and the invariance in law of $\mathbf{z}_\ell^{(ij)}$ under the rotation $\mathbf{z}_\ell^{(ij)} \mapsto \mathbf{u}^\top \mathbf{z}_\ell^{(ij)} \mathbf{u}$ for any orthogonal matrix $\mathbf{u} \in \mathbb{R}^{k_\ell \times k_\ell}$, each observation $\mathbf{y}_\ell^{(ij)}$ is equivalent to observing

$$\tilde{\mathbf{y}}_\ell^{(ij)} = \begin{pmatrix} \phi_{\ell,1}(\mathbf{g}) & & & \\ & \ddots & & \\ & & \phi_{\ell,M}(\mathbf{g}) & \\ & & & \ddots \end{pmatrix}^\top \begin{pmatrix} \phi_{\ell,1}(\mathbf{g}) & & & \\ & \ddots & & \\ & & \phi_{\ell,M}(\mathbf{g}) & \\ & & & \ddots \end{pmatrix} + \tilde{\mathbf{z}}_\ell^{(ij)}$$

where $\phi_{\ell,1}, \dots, \phi_{\ell,M}$ are real-irreducible orthogonal sub-representations of ϕ_ℓ , and $\{\tilde{\mathbf{z}}_\ell^{(ij)}\}$ are standard Gaussian noise matrices equal in law to $\{\mathbf{z}_\ell^{(ij)}\}$. The coordinates of $\tilde{\mathbf{y}}_\ell^{(ij)}$ outside the M diagonal blocks, as well as the coordinates of any diagonal block corresponding to a trivial representation $\phi_{\ell,m}$, carry no information about \mathbf{g} and hence may be discarded. Thus the observation model (21) is equivalent to a model in which each representation ϕ_ℓ is real-irreducible and non-trivial.

If two such representations $\phi_\ell, \phi_{\ell'}$ are isomorphic, then Proposition D.15 implies that there exists an orthogonal matrix $\mathbf{u} \in \mathbb{R}^{k_\ell \times k_{\ell'}}$ for which $\phi_\ell(\mathbf{g}) = \mathbf{u}\phi_{\ell'}(\mathbf{g})\mathbf{u}^\top$. Then, replacing $\{\mathbf{y}_\ell^{(ij)}\}$ by the equivalent observations $\tilde{\mathbf{y}}_\ell^{(ij)} = \mathbf{u}^\top \mathbf{y}_\ell^{(ij)} \mathbf{u}$ as above, we may assume that $\phi_\ell(\mathbf{g}) = \phi_{\ell'}(\mathbf{g})$ for all $\mathbf{g} \in \mathcal{G}$. We may then replace the observations in the two channels $\{\mathbf{y}_\ell^{(ij)}\}$ and $\{\mathbf{y}_{\ell'}^{(ij)}\}$ by their sufficient statistics $\{\frac{\mathbf{y}_\ell^{(ij)} + \mathbf{y}_{\ell'}^{(ij)}}{\sqrt{2}}\}$, which yields a new channel for the representation \mathbf{g}_ℓ having the same standard Gaussian law for the noise, and with a new signal-to-noise parameter $\sqrt{\lambda} = \frac{\sqrt{\lambda_\ell} + \sqrt{\lambda_{\ell'}}}{\sqrt{2}}$. Applying this replacement iteratively, the observation model (21) is then equivalent to a model in which the real-irreducible representations $\{\phi_\ell\}_{\ell=1}^L$ are also distinct.

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