MIMO Channel Shaping and Rate Maximization Using Beyond Diagonal RIS

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***Abstract*—This paper investigates the capability of a passive Reconfigurable Intelligent Surface (RIS) to redistribute the singular values of point-to-point Multiple-Input Multiple-Output (MIMO) channels for achieving power and rate gains. We depart from the conventional Diagonal (D)-RIS with diagonal phase shift matrix and adopt a Beyond Diagonal (BD) architecture that offers greater wave manipulation flexibility through element-wise connections. Specifically, we first provide shaping insights by characterizing the channel singular value regions attainable by D-RIS and BD-RIS via a novel geodesic optimization. Analytical singular value bounds are then derived to explore their shaping limits in typical deployment scenarios. As a side product, we tackle BD-RIS-aided MIMO rate maximization problem by a local-optimal Alternating Optimization (AO) and a shaping-inspired low-complexity approach. Results show that compared to D-RIS, BD-RIS significantly improves the dynamic range of all channel singular values, the trade-off in manipulating them, and thus the channel power and achievable rate. Those observations become more pronounced when the number of RIS elements and MIMO dimensions increase. Of particular interest, BD-RIS is shown to activate multi-stream transmission at lower transmit power than D-RIS, hence achieving the asymptotic Degrees of Freedom (DoF) at low Signal-to-Noise Ratio (SNR) thanks to its higher flexibility of shaping the distribution of channel singular values.**

***Index Terms*—Reconfigurable intelligent surface, channel singular value redistribution, rate maximization, manifold optimization.**

I. Introduction

A. Background

Today we are witnessing a paradigm shift from connectivity to intelligence, where the wireless environment is no longer a chaotic medium but a conscious agent that can serve on demand. This is empowered by recent advances in Reconfigurable Intelligent Surface (RIS), a programmable passive planar surface that recycles and redistributes ambient electromagnetic waves for improved wireless performance. A typical RIS consists of numerous low-power sub-wavelength non-resonant scattering elements, whose response can be engineered in real-time to manipulate the amplitude, phase, frequency, and polarization of the scattered waves [1]. It enables low-noise full-duplex operation, featuring better flexibility than reflectarrays, lighter footprint than relays, and greater scalability than Multiple-Input Multiple-Output (MIMO) systems. One popular RIS research direction is *joint passive and active beamforming* design with transceivers to enhance a specific performance measure, which has attracted significant interests in wireless communication [2]–[4], sensing [5]–[7], and power transfer literature [8]–[10]. While passive beamforming at RIS suffers attenuation from double fading, it offers better asymptotic behaviors than active beamforming at transceivers (e.g., second-order array gain and fourth-order harvested power [10]). Another RIS application is *information modulation* by periodically switching its reflection pattern within the channel coherence time. This creates a free-ride message stream with dual benefits: integrating with legacy transmitter for enhanced channel capacity [11]–[13], or serving as individual source for low-power uplink communication [14]–[16]. Different from above, *channel shaping* exploits RIS as a stand-alone device to modify the inherent properties of the wireless environment, for example, compensate for the Doppler effect [17], flatten frequency-selective channels [18], improve MIMO channel rank [19], and artificially diversify channel over time for orthogonal [20] and non-orthogonal [21] multiple access schemes. This helps to decouple joint beamforming problems into a channel shaping stage and a legacy transceiver design stage, providing a versatile solution for various wireless applications.

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This work has been partially supported by UKRI grant EP/Y004086/1, EP/X040569/1, EP/Y037197/1, EP/X04047X/1, EP/Y037243/1.

B. Related Works

At a specific resource block, channel shaping metrics can be classified into two categories:

- *Singular value:* The impact of RIS has been studied in terms of minimum singular value [22], effective rank [22], [23], condition number [24], [25], and degree of freedom [26]–[28]. Those are closely related to performance measures (e.g., achievable rate and harvested power [29]) but sensitive to minor perturbations of the channel matrix.
- *Power:* The impact of RIS has been studied in terms of channel power gain [2], [30]–[33] in point-to-point channels and leakage interference [34] in interference channels. Those second-order metrics are less informative in MIMO but easier to analyze and optimize.

Although above works offered inspiring glimpses into the channel shaping potential of passive RIS, none attempted to disclose the entire attainable channel singular value region. Most relevant literature [2], [22]–[28], [34] have also been limited to a Diagonal (D)-RIS model where each element is connected to a dedicated impedance and disconnected from others. As such, wave impinging on one element is entirely scattered by the same element. This simple architecture is modeled by a diagonal scattering matrix with unit-magnitude diagonal entries, which only applies a phase shift to the incoming signal. The idea was soon generalized to Beyond Diagonal (BD)-RIS with group-connected architecture [30], where adjacent elements within the same group are connected via passive reconfigurable components[1]. This allows wave impinging on one element to propagate within the circuit and depart partially from any element in the same group. It can thus manipulate both amplitude and phase of the scattered wave while remaining passive. Such a powerful model can be realized at reduced hardware cost using tree- and forest-connected architectures by graph theory [32]. BD-RIS can also function in multi-sector mode [36] for full-space coverage and multi-user support. Practical challenges such as channel estimation [37], mutual coupling [38], and wideband modelling [39] have also been studied in recent literature. Its beamforming superiority over D-RIS has been proved in Single-Input Single-Output (SISO) and Multiple-Input Single-Output (MISO) systems [30]–[33], [36], [40]–[42], however, the interplay between BD-RIS and MIMO is still in the infancy stage. The authors of [43] investigated the rate-optimal joint beamforming design for a fully-connected BD-RIS-aided MIMO system where the direct channel is negligible. A transmitter-side BD-RIS was introduced to massive MIMO systems that exploits statistical Channel State Information (CSI) for improved spectral efficiency [44], which again assumed negligible direct channel and fully-connected BD-RIS. Received power maximization with continuous-valued and discrete-valued BD-RIS have been tackled respectively in closed form [31] and by machine learning approach [45], but the corresponding single-stream transceiver is rate-suboptimal.

C. Contributions

This paper is motivated by a fundamental question: *What is the singular value (and power gain) shaping capability of a passive RIS in point-to-point MIMO channels?* We aim for a comprehensive answer via analysis and optimization. The contributions are summarized below.

First, we pioneer BD-RIS study in general MIMO channels and interpret its shaping potential as branch matching and mode alignment. Branch matching refers to pairing and combining the branches (i.e., entries) of backward and forward channels associated with each BD-RIS group. Mode alignment refers to aligning and ordering the modes (i.e., singular vectors) of indirect channels with those of direct channel. The former is uniquely attributed to the off-diagonal entries of the scattering matrix of BD-RIS.

Second, we propose a novel BD-RIS design method that allows reshaping of the available channels through singular values manipulation. Our Riemannian Conjugate Gradient (RCG) method compares favorably with respect to existing ones in that the updates are along the geodesics (i.e., the shortest path between two points in a Riemannian manifold) of the feasible domain to accelerate convergence. It also works for general design problems of group-connected BD-RIS.

[1]Those components can be either symmetric (e.g., capacitors and inductors) or asymmetric (e.g., ring hybrids and branch-line hybrids) [35], resulting in symmetric and asymmetric scattering matrices, respectively.

Third, we provide a numerical answer to the shaping question by characterizing the Pareto frontiers of channel singular values. The enclosed region generalizes most relevant metrics and provides an intuitive shaping benchmark. Results show that increasing BD-RIS group size enlarges this region, improving the dynamic range of all singular values and the trade-off in manipulating them.

Fourth, we provide an analytical answer to the shaping question in typical deployment scenarios. When the forward/backward channel is rank-deficient, we derive singular value bounds applying to D- and BD-RIS with asymptotically large number of elements. When the direct channel is negligible, we derive singular value bounds applying to fully-connected BD-RIS with arbitrary number of elements. Those bounds are validated by comparing with the numerical results above. Results show that for a fixed number of elements, BD-RIS can approach the asymptotic bounds better than D-RIS.

Fifth, we tackle BD-RIS-aided MIMO rate maximization problem by a local-optimal Alternating Optimization (AO) and a shaping-inspired low-complexity approach. The former iteratively updates active beamforming by eigenmode transmission and passive beamforming by geodesic RCG, until convergence. The latter exploits the BD-RIS to shape the channel for maximum power gain then performs eigenmode transmission. Interestingly, the rate deficit from the shaping-inspired approach diminishes as the BD-RIS evolves towards fully-connected. We conclude that: 1) channel shaping decouples joint beamforming for reduced design complexity; 2) the power and rate gains of BD-RIS over D-RIS increase with the number of scattering elements and MIMO dimensions; 3) at low transmit power, BD-RIS can activate more streams than D-RIS and achieve the asymptotic Degrees of Freedom (DoF), thanks to its higher flexibility of shaping the distribution of channel singular values.

Notation: Italic, bold lower-case, and bold upper-case letters indicate scalars, vectors and matrices, respectively. $\jmath$ denotes the imaginary unit. $\mathbb{H}^{n\times n}$, $\mathbb{H}_{+}^{n\times n}$, and $\mathbb{U}^{n\times n}$ denote the set of $n\times n$ Hermitian, positive semi-definite, and unitary matrices, respectively. $\Re\{\cdot\}$ takes the real part of a complex number. $\mathrm{diag}(\cdot)$ constructs a square matrix with arguments on the main (block) diagonal and zeros elsewhere. $\mathrm{sv}(\cdot)$, $\mathrm{ran}(\cdot)$, and $\ker(\cdot)$ evaluate the singular values (in descending order), column space (range), and kernel of a matrix, respectively. $\mathrm{conv}(\cdot)$ returns the convex hull of arguments. $|\cdot|$, $\|\cdot\|$, and $\|\cdot\|_{\mathrm{F}}$ denote the absolute value, Euclidean norm, and Frobenius norm, respectively. $\sigma_n(\cdot)$ and $\lambda_n(\cdot)$ are the n-th largest singular value and eigenvalue, respectively. $(\cdot)^*$, $(\cdot)^{\mathsf{T}}$, $(\cdot)^{\mathsf{H}}$, $(\cdot)^{\dagger}$, $(\cdot)^{\star}$ denote the conjugate, transpose, conjugate transpose (Hermitian), Moore-Penrose inverse, and stationary point, respectively. $[N]$ is a shortcut for $\{1,2,\dots,N\}$. $(\cdot)_{[x:y]}$ is a shortcut for $(\cdot)_x,(\cdot)_{x+1},\dots,(\cdot)_y$. $\odot$ denotes the element-wise (Hadamard) product. $\mathcal{N}_{\mathbb{C}}(\mathbf{0},\mathbf{\Sigma})$ is the multivariate Circularly Symmetric Complex Gaussian (CSCG) distribution with mean $\mathbf{0}$ and covariance $\mathbf{\Sigma}$. $\sim$ means "distributed as".

II. System Model

A. BD-RIS

The BD-RIS can be modeled as an N_{S}-port network [46] that divides into G individual groups, where group $g\in[G]$

contains N_g scattering elements interconnected by real-time reconfigurable components [30]. Apparently $N_\mathrm{S} = \sum_{g=1}^{G} N_g$. Without loss of generality we assume equal size for all groups $N_g = L \triangleq N_\mathrm{S}/G$, $\forall g$ and no mutual coupling between elements. For asymmetric BD-RIS, the overall scattering matrix is block-diagonal with unitary blocks[2]

$$\mathbf{\Theta} = \mathrm{diag}(\mathbf{\Theta}_1, \ldots, \mathbf{\Theta}_G), \tag{1}$$

where $\mathbf{\Theta}_g \in \mathbb{U}^{L \times L}$ is the g-th diagonal block modeling the response of group g. It is noteworthy that D-RIS is an extreme case of (1) with group size $L = 1$, that is, each element is an individual. Some viable architectures of BD-RIS are illustrated in [30, Fig. 3], [36, Fig. 5], [32, Fig. 2] where the array geometry and circuit topology are modeled in $\mathbf{\Theta}$.

B. MIMO Point-to-Point Channel

Consider a BD-RIS aided MIMO Point-to-Point Channel (PC) with N_T and N_R transmit and receive antennas, respectively, and N_S scattering elements at the BD-RIS. This configuration is denoted as $N_\mathrm{T} \times N_\mathrm{S} \times N_\mathrm{R}$. Let $\mathbf{H}_\mathrm{D} \in \mathbb{C}^{N_\mathrm{R} \times N_\mathrm{T}}$, $\mathbf{H}_\mathrm{B} \in \mathbb{C}^{N_\mathrm{R} \times N_\mathrm{S}}$, $\mathbf{H}_\mathrm{F} \in \mathbb{C}^{N_\mathrm{S} \times N_\mathrm{T}}$ denote the direct (i.e., transmitter-receiver), backward (i.e., RIS-receiver), and forward (i.e., transmitter-RIS) channels, respectively. The equivalent channel depends on the BD-RIS scattering matrix

$$\mathbf{H} = \mathbf{H}_\mathrm{D} + \mathbf{H}_\mathrm{B} \mathbf{\Theta} \mathbf{H}_\mathrm{F} = \mathbf{H}_\mathrm{D} + \sum_g \mathbf{H}_{\mathrm{B},g} \mathbf{\Theta}_g \mathbf{H}_{\mathrm{F},g} \triangleq \mathbf{H}_\mathrm{D} + \sum_g \mathbf{H}_g, \tag{2}$$

where $\mathbf{H}_{\mathrm{B},g} \in \mathbb{C}^{N_\mathrm{R} \times L}$ and $\mathbf{H}_{\mathrm{F},g} \in \mathbb{C}^{L \times N_\mathrm{T}}$ are the backward and forward channels associated with group g, corresponding to the $(g-1)L+1$ to gL columns of $\mathbf{H}_\mathrm{B}$ and rows of $\mathbf{H}_\mathrm{F}$, respectively, and $\mathbf{H}_g \triangleq \mathbf{H}_{\mathrm{B},g} \mathbf{\Theta}_g \mathbf{H}_{\mathrm{F},g}$ is the indirect channel via group g. Since unitary matrices constitute an algebraic group with respect to multiplication, the scattering matrix of group g can be decomposed as

$$\mathbf{\Theta}_g = \mathbf{L}_g \mathbf{R}_g^\mathsf{H}, \tag{3}$$

where $\mathbf{L}_g, \mathbf{R}_g \in \mathbb{U}^{L \times L}$ are two unitary factor matrices. Let $\mathbf{H}_{\mathrm{B/F},g} = \mathbf{U}_{\mathrm{B/F},g} \mathbf{\Sigma}_{\mathrm{B/F},g} \mathbf{V}_{\mathrm{B/F},g}^\mathsf{H}$ be the Singular Value Decomposition (SVD) of the backward and forward channels, respectively. The equivalent channel is thus

$$\mathbf{H} = \overbrace{\mathbf{H}_\mathrm{D} + \sum_g \mathbf{U}_{\mathrm{B},g} \mathbf{\Sigma}_{\mathrm{B},g} \underbrace{\mathbf{V}_{\mathrm{B},g}^\mathsf{H} \mathbf{L}_g \mathbf{R}_g^\mathsf{H} \mathbf{U}_{\mathrm{F},g}}_{\text{backward-forward}} \mathbf{\Sigma}_{\mathrm{F},g} \mathbf{V}_{\mathrm{F},g}^\mathsf{H}}^{\text{direct-indirect}}. \tag{4}$$

Remark 1. In (4), the BD-RIS performs a blockwise unitary transformation to combine the backward-forward (intra-group, multiplicative) channels and direct-indirect (inter-group, additive) channels. These two attributes are refined as:

- *Branch matching:* It refers to pairing and combining the branches (i.e., entries) of $\mathbf{H}_{\mathrm{B},g}$ and $\mathbf{H}_{\mathrm{F},g}$ through $\mathbf{\Theta}_g$.
- *Mode alignment:* It refers to aligning and ordering the modes (i.e., singular vectors) of $\{\mathbf{H}_g\}_{g \in [G]}$ with those of $\mathbf{H}_\mathrm{D}$ through $\{\mathbf{\Theta}_g\}_{g \in [G]}$.

[2]We assume asymmetric network by default to establish a benchmark for passive RIS. Some symmetric solutions (i.e., $\mathbf{\Theta} = \mathbf{\Theta}^\mathsf{T}$) will be discussed and their performance will be evaluated in Section V.

Example 1 (SISO channel gain maximization)**.** Denote the direct, backward, forward channels as h_D, $\mathbf{h}_\mathrm{B} \in \mathbb{C}^{N_\mathrm{S} \times 1}$, and $\mathbf{h}_\mathrm{F}^\mathsf{H} \in \mathbb{C}^{1 \times N_\mathrm{S}}$, respectively. In this case, mode alignment boils down to phase matching and any $L \in [N_\mathrm{S}]$, including D-RIS, suffices for perfect mode alignment using

$$\mathbf{\Theta}_{\text{P-max},g}^{\text{SISO}} = \frac{h_\mathrm{D}}{|h_\mathrm{D}|} \mathbf{V}_{\mathrm{B},g} \mathbf{U}_{\mathrm{F},g}^\mathsf{H}, \quad \forall g, \tag{5}$$

where $\mathbf{V}_{\mathrm{B},g} = \left[\mathbf{h}_{\mathrm{B},g}/\|\mathbf{h}_{\mathrm{B},g}\|, \ \mathbf{N}_{\mathrm{B},g}\right] \in \mathbb{U}^{L \times L}$, $\mathbf{U}_{\mathrm{F},g} = \left[\mathbf{h}_{\mathrm{F},g}/\|\mathbf{h}_{\mathrm{F},g}\|, \mathbf{N}_{\mathrm{F},g}\right] \in \mathbb{U}^{L \times L}$, and $\mathbf{N}_{\mathrm{B/F},g} \in \mathbb{C}^{L \times (L-1)}$ are the orthonormal bases of kernels of $\mathbf{h}_{\mathrm{B/F},g}$. Evidently, the maximum channel gain is a function of L

$$|h|_{\max} = |h_\mathrm{D}| + \sum_g \sum_l |h_{\mathrm{B},g,\pi_{\mathrm{B},g}(l)}| |h_{\mathrm{F},g,\pi_{\mathrm{F},g}(l)}|, \tag{6}$$

where $h_{\mathrm{B/F},g,l}$ are the l-th entries of $\mathbf{h}_{\mathrm{B/F},g}$, and $\pi_{\mathrm{B/F},g}$ are permutations of $[L]$ sorting their magnitude in similar orders. That is, the maximum SISO channel gain is attained when each BD-RIS group, apart from phase shifting, matches the l-th strongest backward and forward channel branches therein. A larger L provides more flexible branch matching and thus higher channel gain.

Example 1 clarifies the difference between branch matching and mode alignment and show their impacts on channel shaping. When it comes to MIMO, the advantage of BD-RIS in branch matching improves since the number of available branches is proportional to $N_\mathrm{T} N_\mathrm{R}$. On the other hand, the limitation of D-RIS in mode alignment worsens since each element can only apply a phase shift to the indirect channel of $N \triangleq \min(N_\mathrm{T}, N_\mathrm{R})$ modes.

C. MIMO Interference Channel

We also consider a BD-RIS aided MIMO Interference Channel (IC) of K transceiver pairs where each transmitter and receiver has N_T and N_R antennas, respectively, and the BD-RIS has N_S scattering elements. This configuration is denoted as $(N_\mathrm{T} \times N_\mathrm{S} \times N_\mathrm{R})^K$. Let $\mathbf{H}_\mathrm{D}^{(kj)} \in \mathbb{C}^{N_\mathrm{R} \times N_\mathrm{T}}$, $\mathbf{H}_\mathrm{B}^{(k)} \in \mathbb{C}^{N_\mathrm{R} \times N_\mathrm{S}}$, $\mathbf{H}_\mathrm{F}^{(j)} \in \mathbb{C}^{N_\mathrm{S} \times N_\mathrm{T}}$ denote the direct channel from transmitter j to receiver k, the backward channel of receiver k, and the forward channel of transmitter j, respectively, where $(j,k) \in [K]^2$. Assume all transmitter-RIS-receiver paths share the same BD-RIS scattering matrix $\mathbf{\Theta}$. The equivalent channel from transmitter j to receiver k is

$$\mathbf{H}^{(kj)} = \mathbf{H}_\mathrm{D}^{(kj)} + \mathbf{H}_\mathrm{B}^{(k)} \mathbf{\Theta} \mathbf{H}_\mathrm{F}^{(j)} = \mathbf{H}_\mathrm{D}^{(kj)} + \sum_g \mathbf{H}_{\mathrm{B},g}^{(k)} \mathbf{\Theta}_g \mathbf{H}_{\mathrm{F},g}^{(j)}, \tag{7}$$

where $\mathbf{H}_{\mathrm{B},g}^{(k)} \in \mathbb{C}^{N_\mathrm{R} \times L}$ and $\mathbf{H}_{\mathrm{F},g}^{(j)} \in \mathbb{C}^{L \times N_\mathrm{T}}$ are associated with RIS group g, corresponding to the $(g-1)L+1$ to gL columns of $\mathbf{H}_{\mathrm{B},g}^{(k)}$ and rows of $\mathbf{H}_{\mathrm{F},g}^{(j)}$, respectively,

III. Channel Shaping

In this section, we first provide an example demonstrating the MIMO channel shaping advantages of BD-RIS over D-RIS, then derive some analytical bounds related to channel singular values under specific channel conditions, and provide closed-form BD-RIS solution for several cases of interest.

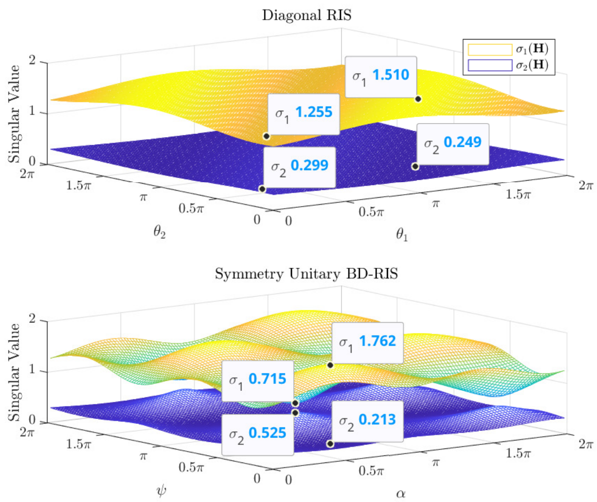


Fig. 1. $2 \times 2 \times 2$ singular value shaping by D-RIS and symmetric fully-connected BD-RIS when the direct channel is negligible. $\sigma_1(\mathbf{H})$ and $\sigma_2(\mathbf{H})$ refer to the most and least dominant singular values, respectively. Their maximum and minimum are marked explicitly on the plot.

Finally, we propose a numerical method to optimize the BD-RIS for a special class of singular value function under general channel conditions.

Example 2 ($2 \times 2 \times 2$ shaping)**.** Here D-RIS and fully-connected BD-RIS can be modeled by 2 and 4 independent angular parameters, respectively:

$$\mathbf{\Theta}_{\mathrm{D}} = \mathrm{diag}(e^{\jmath\theta_1}, e^{\jmath\theta_2}), \quad \mathbf{\Theta}_{\mathrm{BD}} = e^{\jmath\phi}\begin{bmatrix} e^{\jmath\alpha}\cos\psi & e^{\jmath\beta}\sin\psi \\ -e^{-\jmath\beta}\sin\psi & e^{-\jmath\alpha}\cos\psi \end{bmatrix},$$

We restrict the discussion to a special case where the BD-RIS is symmetric (i.e., $\beta=\pi/2$) and the direct channel is negligible such that ϕ has no impact on $\mathrm{sv}(\mathbf{H})$, since $\mathrm{sv}(e^{\jmath\phi}\mathbf{A})=\mathrm{sv}(\mathbf{A})$. The singular value shaping capabilities of $\mathbf{\Theta}_{\mathrm{D}}$ and $\mathbf{\Theta}_{\mathrm{BD}}$ can thus be compared visually over 2 tunable parameters. With an exhaustive grid search over (θ_1,θ_2) and (α,ψ), Fig. 1 shows the achievable singular values of a specific channel realization

$$\mathbf{H}_{\mathrm{B}} = \begin{bmatrix} -0.2059+0.5914\jmath & -0.0909+0.5861\jmath \\ 0.4131+0.2651\jmath & -0.1960+0.4650\jmath \end{bmatrix},$$

$$\mathbf{H}_{\mathrm{F}} = \begin{bmatrix} -0.6362+0.1332\jmath & -0.1572+1.5538\jmath \\ 0.0196+0.4011\jmath & -0.3170-0.2303\jmath \end{bmatrix}.$$

In this example, both singular values can be manipulated up to[3] $\pm 9\%$ by D-RIS and $\pm 42\%$ by symmetric fully-connected BD-RIS. It is noteworthy that the former requires 2 circuit components and the latter requires 3.

Example 2 suggests that the physical interconnection of RIS elements, even if using symmetric circuit components, can create a "cooperation effect" that significantly enhances the dynamic range of channel singular values. This motivates the analytical and numerical channel shaping studies in Section III-A and III-B, respectively.

[3]The percentage for manipulating $\sigma_n(\mathbf{H})$ is calculated by $\eta_n^+ = \frac{\max\sigma_n(\mathbf{H})-\mathrm{avg}\sigma_n(\mathbf{H})}{\mathrm{avg}\sigma_n(\mathbf{H})} \times 100\%$ and $\eta_n^- = \frac{\min\sigma_n(\mathbf{H})-\mathrm{avg}\sigma_n(\mathbf{H})}{\mathrm{avg}\sigma_n(\mathbf{H})} \times 100\%$.

A. Analytical Shaping Bounds

The main results of this subsection are presented in the following Propositions and Corollaries.

Proposition 1 (Degrees of freedom)**.** *BD-RIS may achieve a larger or smaller number of MIMO DoF[4] than D-RIS.*

Proof. Please refer to Appendix A. □

Proposition 1 suggests that we can expect more parallel streams or less interference when shaping the channel with BD-RIS. We now take a step further to examine the limits of redistributing channel singular values under specific channel conditions.

Proposition 2 (Rank-deficient channel)**.** *If the minimum rank of backward and forward channels is k ($k \leq N$), then for D-RIS or BD-RIS of arbitrary number of elements, the n-th singular value of the equivalent channel is bounded above and below respectively by*

$$\sigma_n(\mathbf{H}) \leq \sigma_{n-k}(\mathbf{T}), \qquad \text{if } n>k, \tag{8a}$$

$$\sigma_n(\mathbf{H}) \geq \sigma_n(\mathbf{T}), \qquad \text{if } n<N-k+1, \tag{8b}$$

where $\mathbf{T}$ is arbitrary auxiliary matrix satisfying

$$\mathbf{T}\mathbf{T}^{\mathsf{H}} = \begin{cases} \mathbf{H}_{\mathrm{D}}(\mathbf{I}-\mathbf{V}_{\mathrm{F}}\mathbf{V}_{\mathrm{F}}^{\mathsf{H}})\mathbf{H}_{\mathrm{D}}^{\mathsf{H}}, & \text{if } \mathrm{rank}(\mathbf{H}_{\mathrm{F}})=k, \\ \mathbf{H}_{\mathrm{D}}^{\mathsf{H}}(\mathbf{I}-\mathbf{U}_{\mathrm{B}}\mathbf{U}_{\mathrm{B}}^{\mathsf{H}})\mathbf{H}_{\mathrm{D}}, & \text{if } \mathrm{rank}(\mathbf{H}_{\mathrm{B}})=k, \end{cases} \tag{9}$$

and $\mathbf{V}_{\mathrm{F}}$ and $\mathbf{U}_{\mathrm{B}}$ are any right and left singular matrices of $\mathbf{H}_{\mathrm{F}}$ and $\mathbf{H}_{\mathrm{B}}$, respectively.

Proof. Please refer to Appendix B. □

Inequality (8a) states that if $\mathbf{H}_{\mathrm{B}}$ and $\mathbf{H}_{\mathrm{F}}$ are at least rank k, then with a D-RIS or BD-RIS of sufficiently large N_{S}, the n-th singular value of $\mathbf{H}$ can be enlarged to the $(n-k)$-th singular value of $\mathbf{T}$, or suppressed to the n-th singular value of $\mathbf{T}$. Moreover, the first k channel singular values are unbounded above[5] while the last k channel singular values can be suppressed to zero. A special case is Corollary 2.1 for Line-of-Sight (LoS) channel[6].

Corollary 2.1 (LoS channel)**.** *If at least one of backward and forward channels is LoS, then a D-RIS or BD-RIS can at most enlarge the n-th ($n \geq 2$) channel singular value to the $(n-1)$-th singular value of $\mathbf{T}$, or suppress the n-th channel singular value to the n-th singular value of $\mathbf{T}$. That is,*

$$\sigma_1(\mathbf{H}) \geq \sigma_1(\mathbf{T}) \geq \sigma_2(\mathbf{H}) \geq \ldots \geq \sigma_{N-1}(\mathbf{T}) \geq \sigma_N(\mathbf{H}) \geq \sigma_N(\mathbf{T}). \tag{10}$$

Proof. This is a direct result of (8) with $k=1$. □

We emphasize that Proposition 2 and Corollary 2.1 apply to both D- and BD-RIS configurations regardless of the status of the direct channel. Out of $2N$ bounds in (8) or (10), N of them can be *simultaneously* tight as $N_{\mathrm{S}} \to \infty$, namely, when the

[4]DoF refers to the maximum number of independent streams that can be transmitted in parallel over a MIMO channel. It is defined as $\mathrm{DoF}(\mathbf{H}) = \lim_{\rho\to\infty} \frac{\log\det(\mathbf{I}+\rho\mathbf{H}\mathbf{H}^{\mathsf{H}})}{\log\rho}$ where ρ is the Signal-to-Noise Ratio (SNR).

[5]The energy conservation law $\sum_{n=1}^{N}\sigma_n^2(\mathbf{H}) \leq 1$ still has to be respected in all cases. This constraint is omitted in context for brevity.

[6]A similar eigenvalue result has been derived for D-RIS only [47].

direct channel becomes negligible[7]. For a finite N_{S}, the RIS may prioritize a subset of those by aligning the corresponding modes, and we will later show by simulation that BD-RIS outperforms D-RIS on this purpose. Proposition 2 provides a reference on the selection of N_{S} in low-multipath application scenarios. Next, we shift the focus to another popular RIS deployment scenario where the direct channel is blocked.

Proposition 3 (Negligible direct channel)**.** *If the direct channel is negligible, then a fully-connected BD-RIS can manipulate the channel singular values up to*

$$\mathrm{sv}(\mathbf{H}) = \mathrm{sv}(\mathbf{B}\mathbf{F}), \tag{11}$$

where $\mathbf{B}$ *and* $\mathbf{F}$ *are arbitrary matrices with* $\mathrm{sv}(\mathbf{B}) = \mathrm{sv}(\mathbf{H}_{\mathrm{B}})$ *and* $\mathrm{sv}(\mathbf{F}) = \mathrm{sv}(\mathbf{H}_{\mathrm{F}})$.

Proof. Please refer to Appendix C. □

Proposition 3 says that if the direct channel is negligible and the BD-RIS is fully-connected, the only singular value bounds on the equivalent channel are those on the product of unitary-transformed backward and forward channels. It is *not necessarily* an asymptotic result and does *not* depend on any relationship between N_{R}, N_{S}, and N_{T}. Its importance lies in the fact that our initial channel shaping question can be recast as a linear algebra question: *How the singular values of matrix product are bounded by the singular values of its individual factors?* The question is partially answered in Corollaries 3.1–3.3 over definition[8] $\bar{N} = \max(N_{\mathrm{T}}, N_{\mathrm{S}}, N_{\mathrm{R}})$ and $\sigma_n(\mathbf{H}) = \sigma_n(\mathbf{H}_{\mathrm{F}}) = \sigma_n(\mathbf{H}_{\mathrm{B}}) = 0$, $\forall n \in [\bar{N}] \setminus [N]$. The results are by no means complete and interested readers are referred to [48, Chapter 16, 24] and [49, Chapter 3] for more information.

Corollary 3.1 (Product of subset of singular values)**.** *If the direct channel is negligible, then the product of subset of singular values of* $\mathbf{H}$ *is bounded from above by those of* $\mathbf{H}_{\mathrm{B}}$ *and* $\mathbf{H}_{\mathrm{F}}$*, that is,*

$$\prod_{k\in K} \sigma_k(\mathbf{H}) \leq \prod_{i\in I} \sigma_i(\mathbf{H}_{\mathrm{B}}) \prod_{j\in J} \sigma_j(\mathbf{H}_{\mathrm{F}}), \tag{12}$$

for all admissible triples $(I,J,K) \in T_r^{\bar{N}}$ *with* $r < \bar{N}$*, where*

$$T_r^{\bar{N}} \triangleq \Big\{ (I,J,K) \in U_r^{\bar{N}} \,\Big|\, \forall p < r,\ \forall (F,G,H) \in T_p^r, \\ \sum_{f\in F} i_f + \sum_{g\in G} j_g \leq \sum_{h\in H} k_h + \frac{p(p+1)}{2} \Big\},$$

$$U_r^{\bar{N}} \triangleq \Big\{ (I,J,K) \subseteq [\bar{N}]^3 \,\Big|\, \sum_{i\in I} i + \sum_{j\in J} j = \sum_{k\in K} k + \frac{r(r+1)}{2} \Big\}.$$

Proof. Please refer to [50, Theorem 8]. □

Inequality (12), also recognized as a variation of Horn's inequality [51], is one of the most comprehensive result over Proposition 3. However, the number of admissible triples increases exponentially[9] with N_{S} despite some resulting bounds can be redundant. We will shortly see (12) can also induce lower bounds on channel singular values. Those facts render the shaping limit analysis non-trivial for large-scale RIS-aided MIMO systems. Below we showcase some useful bounds therein.

Corollary 3.2 (Product of some largest or smallest singular values)**.** *If the direct channel is negligible, then the product of the first (resp. last*[10]*)* k *singular values of* $\mathbf{H}$ *is bounded from above (resp. below) by those of* $\mathbf{H}_{\mathrm{B}}$ *and* $\mathbf{H}_{\mathrm{F}}$*, that is,*

$$\prod_{n=1}^{k} \sigma_n(\mathbf{H}) \leq \prod_{n=1}^{k} \sigma_n(\mathbf{H}_{\mathrm{B}}) \sigma_n(\mathbf{H}_{\mathrm{F}}), \tag{13a}$$

$$\prod_{n=\bar{N}}^{\bar{N}-k+1} \sigma_n(\mathbf{H}) \geq \prod_{n=\bar{N}}^{\bar{N}-k+1} \sigma_n(\mathbf{H}_{\mathrm{B}}) \sigma_n(\mathbf{H}_{\mathrm{F}}). \tag{13b}$$

Proof. Please refer to Appendix D. □

Corollary 3.3 (Individual singular value)**.** *If the direct channel is negligible, then the* n*-th channel singular value can be manipulated up to*

$$\max_{i+j=n+N_{\mathrm{S}}} \sigma_i(\mathbf{H}_{\mathrm{B}}) \sigma_j(\mathbf{H}_{\mathrm{F}}) \leq \sigma_n(\mathbf{H}) \leq \min_{i+j=n+1} \sigma_i(\mathbf{H}_{\mathrm{B}}) \sigma_j(\mathbf{H}_{\mathrm{F}}), \tag{14}$$

where $(i,j) \in [N_{\mathrm{S}}]^2$*. The upper and lower bounds are attained respectively at*

$$\mathbf{\Theta}_{\text{sv-}n\text{-max}}^{\text{MIMO-ND}} = \mathbf{V}_{\mathrm{B}} \mathbf{P} \mathbf{U}_{\mathrm{F}}^{\mathsf{H}}, \tag{15a}$$

$$\mathbf{\Theta}_{\text{sv-}n\text{-min}}^{\text{MIMO-ND}} = \mathbf{V}_{\mathrm{B}} \mathbf{Q} \mathbf{U}_{\mathrm{F}}^{\mathsf{H}}, \tag{15b}$$

where $\mathbf{V}_{\mathrm{B}}, \mathbf{U}_{\mathrm{F}} \in \mathbb{U}^{N_{\mathrm{S}} \times N_{\mathrm{S}}}$ *are any right and left singular matrices*[11] *of* $\mathbf{H}_{\mathrm{B}}$ *and* $\mathbf{H}_{\mathrm{F}}$*, respectively, and* $\mathbf{P}$ *and* $\mathbf{Q}$ *are arbitrary permutation matrices of dimension* N_{S} *satisfying:*

- *The* (i,j)*-th entry is* 1*, where*

$$(i,j) = \begin{cases} \underset{i+j=n+1}{\arg\min}\ \sigma_i(\mathbf{H}_{\mathrm{B}}) \sigma_j(\mathbf{H}_{\mathrm{F}}) & \textit{for } \mathbf{P}, \quad (16a) \\ \underset{i+j=n+N_{\mathrm{S}}}{\arg\max}\ \sigma_i(\mathbf{H}_{\mathrm{B}}) \sigma_j(\mathbf{H}_{\mathrm{F}}) & \textit{for } \mathbf{Q}, \quad (16b) \end{cases}$$

  and ties may be broken arbitrarily;
- *After deleting the* i*-th row and* j*-th column, the resulting submatrix* $\mathbf{Y}$ *is arbitrary permutation matrix of dimension* $N_{\mathrm{S}}-1$ *satisfying*

$$\sigma_{n-1}(\hat{\mathbf{\Sigma}}_{\mathrm{B}} \mathbf{Y} \hat{\mathbf{\Sigma}}_{\mathrm{F}}) \geq \min_{i+j=n+1} \sigma_i(\mathbf{H}_{\mathrm{B}}) \sigma_j(\mathbf{H}_{\mathrm{F}}) \ \textit{for } \mathbf{P}, \tag{17a}$$

$$\sigma_{n+1}(\hat{\mathbf{\Sigma}}_{\mathrm{B}} \mathbf{Y} \hat{\mathbf{\Sigma}}_{\mathrm{F}}) \leq \max_{i+j=n+N_{\mathrm{S}}} \sigma_i(\mathbf{H}_{\mathrm{B}}) \sigma_j(\mathbf{H}_{\mathrm{F}}) \ \textit{for } \mathbf{Q}, \tag{17b}$$

  where $\hat{\mathbf{\Sigma}}_{\mathrm{B}}$ *and* $\hat{\mathbf{\Sigma}}_{\mathrm{F}}$ *are diagonal singular value matrices of* $\mathbf{H}_{\mathrm{B}}$ *and* $\mathbf{H}_{\mathrm{F}}$ *with both* i*-th row and* j*-th column deleted, respectively.*

Proof. Please refer to Appendix E. □

[7]Negligible direct channel refers to the case where the power of the signal arriving at the receiver through the direct path is negligible compared to that through the scattering of RIS, i.e., $\mathbf{H} \approx \sum_g \mathbf{H}_g$. This can result from a very large number of RIS elements (as discussed in Proposition 2) or physical obstacles in the propagation path (as discussed in Proposition 3).

[8]This is equivalent to padding zero blocks at the end of $\mathbf{H}, \mathbf{H}_{\mathrm{B}}, \mathbf{H}_{\mathrm{F}}$ to make square matrices of dimension $\bar{N}$.

[9]For example, the number of inequalities described by (12) grows from 12 to 2062 when N_{S} increases from 3 to 7.

[10]The lower bounds coincide at zero when $N \neq N$ (i.e., $N_{\mathrm{T}} = N_{\mathrm{S}} = N_{\mathrm{R}}$ being false).

[11] We highlight the non-uniqueness of $\mathbf{V}_{\mathrm{B}}$ and $\mathbf{U}_{\mathrm{F}}$. When a singular value has multiplicity k, the corresponding singular vectors can be any orthonormal basis of the k-dimensional subspace. Even if all singular values are distinct, the singular vectors of each can be scaled by a phase factor of choice.

Corollary 3.3 and Proposition 2 both reveal the shaping limits of individual channel singular values. They are derived under different assumptions are not special cases of each other. Importantly, Corollary 3.3 establishes upper and lower bounds for *each* channel singular value (c.f. first and last few in Proposition 2), applies to fully-connected BD-RIS of arbitrary size, and provides a general solution structure. We emphasize that in (15) the mode alignment is realized by $\mathbf{V}_{\mathrm{B}}$ and $\mathbf{U}_{\mathrm{F}}$ while the ordering is enabled by permutation matrices $\mathbf{P}$ and $\mathbf{Q}$, which are special cases of unitary $\mathbf{X}$ defined in (61). Specially, the extreme channel singular values can be manipulated up to

$$\max_{i+j=N_{\mathrm{S}}+1} \sigma_i(\mathbf{H}_{\mathrm{B}})\sigma_j(\mathbf{H}_{\mathrm{F}}) \leq \sigma_1(\mathbf{H}) \leq \sigma_1(\mathbf{H}_{\mathrm{B}})\sigma_1(\mathbf{H}_{\mathrm{F}}), \tag{18a}$$

$$\min_{i+j=\bar{N}+1} \sigma_i(\mathbf{H}_{\mathrm{B}})\sigma_j(\mathbf{H}_{\mathrm{F}}) \geq \sigma_{\bar{N}}(\mathbf{H}) \geq \sigma_{\bar{N}}(\mathbf{H}_{\mathrm{B}})\sigma_{\bar{N}}(\mathbf{H}_{\mathrm{F}}). \tag{18b}$$

We notice that the right halves in (18a) and (18b) are special cases of (13a) and (13b) when $k=1$.

Example 3 (Bounds on $3\times3\times3$ shaping)**.** Consider a $3\times3\times3$ setup with $\mathbf{H}_{\mathrm{D}}=\mathbf{0}$, $\mathbf{H}_{\mathrm{B}}=\mathrm{diag}(3,2,1)$, and $\mathbf{H}_{\mathrm{F}}=\mathrm{diag}(4,0,5)$.

- D-RIS: It is evident that any D-RIS can only achieve $\mathrm{sv}(\mathbf{H}) = [12, 5, 0]^{\mathsf{T}}$ due to limited branch matching and mode alignment capability.
- BD-RIS: According to (14), a fully-connected BD-RIS can manipulate the singular values up to

  $$8 \leq \sigma_1(\mathbf{H}) \leq 15, \quad 4 \leq \sigma_2(\mathbf{H}) \leq 10, \quad 0 \leq \sigma_3(\mathbf{H}) \leq 0.$$

  To attain the upper and lower bounds, (i,j) in (15a) and (15b) takes $(1,1)$ and $(2,2)$ when $n=1$, and $(2,1)$ and $(3,2)$ when $n=2$, respectively.

We conclude from Example 3 that a fully-connected BD-RIS can widen the dynamic range of channel singular values by properly aligning and ordering the modes of $\mathbf{H}_{\mathrm{B}}$ and $\mathbf{H}_{\mathrm{F}}$. However, when the problem of interest is a function of multiple singular values, their individual bounds (14) may not be simultaneously tight. Some case studies are presented below.

Corollary 3.4 (Channel power gain)**.** *If the direct channel is negligible, then the channel power gain is bounded from above (resp. below) by the inner product of squared singular values of $\mathbf{H}_{\mathrm{B}}$ and $\mathbf{H}_{\mathrm{F}}$ when they are sorted similarly (resp. oppositely), that is,*

$$\sum_{n=1}^{N} \sigma_n^2(\mathbf{H}_{\mathrm{B}})\sigma_{N_{\mathrm{S}}-n+1}^2(\mathbf{H}_{\mathrm{F}}) \leq \|\mathbf{H}\|_{\mathrm{F}}^2 \leq \sum_{n=1}^{N} \sigma_n^2(\mathbf{H}_{\mathrm{B}})\sigma_n^2(\mathbf{H}_{\mathrm{F}}), \tag{19}$$

whose[12] *upper and lower bounds are attained respectively at*

$$\mathbf{\Theta}_{\text{P-max}}^{\text{MIMO-ND}} = \mathbf{V}_{\mathrm{B}}\mathbf{U}_{\mathrm{F}}^{\mathsf{H}}, \tag{20a}$$

$$\mathbf{\Theta}_{\text{P-min}}^{\text{MIMO-ND}} = \mathbf{V}_{\mathrm{B}}\mathbf{J}\mathbf{U}_{\mathrm{F}}^{\mathsf{H}}, \tag{20b}$$

where $\mathbf{J}$ is the exchange (a.k.a. backward identity) matrix of dimension N_{S}.

Proof. Please refer to Appendix F. □

[12]As a side note, we notice [52] discussed a similar bound using extreme singular values $\max\big(\sigma_N(\mathbf{H}_{\mathrm{B}})\|\mathbf{H}_{\mathrm{F}}\|_{\mathrm{F}}^2, \sigma_N(\mathbf{H}_{\mathrm{F}})\|\mathbf{H}_{\mathrm{B}}\|_{\mathrm{F}}^2\big) \leq \|\mathbf{H}\|_{\mathrm{F}}^2 \leq \min\big(\sigma_1(\mathbf{H}_{\mathrm{B}})\|\mathbf{H}_{\mathrm{F}}\|_{\mathrm{F}}^2, \sigma_1(\mathbf{H}_{\mathrm{F}})\|\mathbf{H}_{\mathrm{B}}\|_{\mathrm{F}}^2\big)$. This is a looser version of (19) and cannot take equalities unless the extreme singular values are of multiplicity N.

We notice that (20a) and (20b) are special cases of (15a) and (15b) with $\mathbf{P}=\mathbf{I}$ and $\mathbf{Q}=\mathbf{J}$, which also attain the right and left halves of (18), respectively. As a side note, when both $\mathbf{H}_{\mathrm{B}}$ and $\mathbf{H}_{\mathrm{F}}$ follow Rayleigh fading, the expectation of maximum channel power gain can be numerically evaluated as

$$\mathbb{E}\{\|\mathbf{H}\|_{\mathrm{F}}^2\} = \sum_{n=1}^{N} \int_0^{\infty} x f_{\lambda_n^{\min(N_{\mathrm{R}},N_{\mathrm{S}})}}(x)dx \times \int_0^{\infty} y f_{\lambda_n^{\min(N_{\mathrm{S}},N_{\mathrm{T}})}}(y)dy, \tag{21}$$

where λ_n^K is the n-th eigenvalue of the complex $K\times K$ Wishart matrix with probability density function $f_{\lambda_n^K}(\cdot)$ given by [53, (51)]. (21) generalizes the SISO channel power gain aided by BD-RIS [30, (58)] to MIMO under double Rayleigh fading, but a closed-form expression seems nontrivial. The next corollary has been derived in [43] independently from Proposition 3 and we include it here for completeness of results.

Corollary 3.5 (Channel capacity at general SNR)**.** *If the direct channel is negligible, then the BD-RIS aided MIMO channel capacity is*

$$C^{\text{MIMO-ND}} = \sum_{n=1}^{N} \log\left(1 + \frac{s_n \sigma_n^2(\mathbf{H}_{\mathrm{B}})\sigma_n^2(\mathbf{H}_{\mathrm{F}})}{\eta}\right), \tag{22}$$

where η is the average noise power, $s_n = \mu - \frac{\eta}{\sigma_n^2(\mathbf{H}_{\mathrm{B}})\sigma_n^2(\mathbf{H}_{\mathrm{F}})}$ is the power allocated to the n-th mode obtainable by the water-filling algorithm [54]. The capacity-achieving BD-RIS scattering matrix is

$$\mathbf{\Theta}_{\text{R-max}}^{\text{MIMO-ND}} = \mathbf{V}_{\mathrm{B}}\mathbf{U}_{\mathrm{F}}^{\mathsf{H}}. \tag{23}$$

Proof. Please refer to [43, Appendix A]. □

Corollary 3.5 also suggests that the power- and rate-optimal scattering matrices (20a) and (23) coincide with each other when the direct channel is negligible and the BD-RIS is fully-connected. When either condition is not satisfied, active and passive beamforming are coupled and the rate-optimal solution involves alternating optimization. However, the power-optimal RIS still provides for a low-complexity decoupled solution. The details will be discussed in Section IV-A.

Corollary 3.6 (Channel capacity at extreme SNR)**.** *If the direct channel is negligible, then the channel capacity when the SNR ρ is very low and high are approximately bounded from above by*

$$C_{\rho_\downarrow} \lessapprox \sigma_1^2(\mathbf{H}_{\mathrm{B}})\sigma_1^2(\mathbf{H}_{\mathrm{F}}), \tag{24a}$$

$$C_{\rho_\uparrow} \lessapprox N \log\frac{\rho}{N} + 2\log\prod_{n=1}^{N} \sigma_n(\mathbf{H}_{\mathrm{B}})\sigma_n(\mathbf{H}_{\mathrm{F}}). \tag{24b}$$

Proof. Please refer to Appendix G. □

The ergodic counterparts of (22) and (24) when both $\mathbf{H}_{\mathrm{B}}$ and $\mathbf{H}_{\mathrm{F}}$ follow Rayleigh fading can be evaluated similarly to (21). Proposition 1–3 and the resulting Corollaries provide a partial answer to the channel shaping question in terms of singular values and their functions. Extending the analysis to more general cases (e.g., non-negligible direct channel and arbitrary BD-RIS group size) is non-trivial due to limited branch matching and mode alignment capabilities therein. A numerical solution will be discussed in Section III-B.

B. Numerical Shaping Solution

Consider a special class of channel shaping problem

$$\max_{\mathbf{\Theta}} \quad f\big(\mathrm{sv}(\mathbf{H})\big) \tag{25a}$$
$$\text{s.t.} \quad \mathbf{\Theta}_g^{\mathsf{H}}\mathbf{\Theta}_g = \mathbf{I}, \quad \forall g, \tag{25b}$$

where $f : \mathbb{R}^N \to \mathbb{R}$ is a symmetric gauge function (i.e., a norm invariant under sign change and argument permutation) [55]. Examples of such f include the Ky Fan k norm, Schatten p norm, n-th singular value, and channel power gain. Problem (25) is non-convex due to the unitary constraints (25b).

Proposition 4. *The sub-differential of* (25a) *with respect to BD-RIS block g is*

$$\partial_{\mathbf{\Theta}_g^*} f\big(\mathrm{sv}(\mathbf{H})\big) = \mathrm{conv}\big\{\mathbf{H}_{\mathrm{B},g}^{\mathsf{H}}\mathbf{U}\mathbf{D}\mathbf{V}^{\mathsf{H}}\mathbf{H}_{\mathrm{F},g}^{\mathsf{H}}\big\}, \tag{26}$$

where $\mathbf{D} \in \mathbb{C}^{N_\mathrm{R}\times N_\mathrm{T}}$ is a rectangular diagonal matrix with $[\mathbf{D}]_{n,n} \in \partial_{\sigma_n(\mathbf{H})} f\big(\mathrm{sv}(\mathbf{H})\big)$, $\forall n \in [N]$, and $\mathbf{U}$, $\mathbf{V}$ are any left and right singular matrices of $\mathbf{H}$.

Proof. Please refer to Appendix H. □

With Proposition 4, one can apply the *relax-then-project* method [30], [40] or *non-geodesic*[13] *RCG* [36], [41], [56] to solve Problem (25). The former solves unconstrained problem (25a) by quasi-Newton methods and projects the solution back to domain (25b) without guarantee of optimality. The latter generalizes the conjugate gradient methods to Riemannian manifolds and updates the solution by addition and retraction, which constitutes a zigzag path departing from and returning to the manifold. Next, we introduce a group-wise *geodesic RCG* method modified from [57], [58] that performs multiplicative updates along the geodesics on the Stiefel manifold for faster convergence. It is applicable to a wide range of BD-RIS design problems where the objective f is smooth or convex non-smooth[14] and the only constraint is group-wise unitarity (25b). The steps for updating $\mathbf{\Theta}_g$ at iteration r are summarized below:

1) *Compute the Euclidean (sub-)gradient at $\mathbf{\Theta}_g^{(r)}$:* The (sub-)gradient of f with respect to $\mathbf{\Theta}_g$ in the Euclidean space is

$$\nabla_{\mathrm{E},g}^{(r)} = 2\frac{\partial f(\mathbf{\Theta}_g^{(r)})}{\partial \mathbf{\Theta}_g^*}; \tag{27}$$

2) *Translate to the Riemannian (sub-)gradient at $\mathbf{\Theta}_g^{(r)}$:* At point $\mathbf{\Theta}_g^{(r)}$, the Riemannian (sub-)gradient gives the steepest ascent direction on the manifold. It lies in the tangent space of the manifold $\mathcal{T}_{\mathbf{\Theta}_g^{(r)}}\mathbb{U}^{L\times L} \triangleq \{\mathbf{M}\in\mathbb{C}^{L\times L} \mid \mathbf{M}^{\mathsf{H}}\mathbf{\Theta}_g^{(r)} + \mathbf{\Theta}_g^{(r)\mathsf{H}}\mathbf{M} = \mathbf{0}\}$ and is obtainable by projection:

$$\nabla_{\mathrm{R},g}^{(r)} = \nabla_{\mathrm{E},g}^{(r)} - \mathbf{\Theta}_g^{(r)}\nabla_{\mathrm{E},g}^{(r)\mathsf{H}}\mathbf{\Theta}_g^{(r)}; \tag{28}$$

3) *Translate to the Riemannian (sub-)gradient at the identity:* The Riemannian (sub-)gradient should be translated back to the identity for exploiting the Lie algebra[15]:

$$\tilde{\nabla}_{\mathrm{R},g}^{(r)} = \nabla_{\mathrm{R},g}^{(r)}\mathbf{\Theta}_g^{(r)\mathsf{H}} = \nabla_{\mathrm{E},g}^{(r)}\mathbf{\Theta}_g^{(r)\mathsf{H}} - \mathbf{\Theta}_g^{(r)}\nabla_{\mathrm{E},g}^{(r)\mathsf{H}}. \tag{29}$$

4) *Determine the conjugate direction:* The conjugate direction is obtained over the Riemannian (sub-)gradient and previous direction as

$$\mathbf{D}_g^{(r)} = \tilde{\nabla}_{\mathrm{R},g}^{(r)} + \gamma_g^{(r)}\mathbf{D}_g^{(r-1)}, \tag{30}$$

where $\gamma_g^{(r)}$ is the parameter that deviates the conjugate direction from the tangent space for accelerated convergence. A popular choice is the Polak-Ribière formula [59]

$$\gamma_g^{(r)} = \frac{\mathrm{tr}\big((\tilde{\nabla}_{\mathrm{R},g}^{(r)} - \tilde{\nabla}_{\mathrm{R},g}^{(r-1)})\tilde{\nabla}_{\mathrm{R},g}^{(r)\mathsf{H}}\big)}{\mathrm{tr}\big(\tilde{\nabla}_{\mathrm{R},g}^{(r-1)}\tilde{\nabla}_{\mathrm{R},g}^{(r-1)\mathsf{H}}\big)}. \tag{31}$$

5) *Evaluate the geodesic at the identity:* The geodesic emanating from the identity with velocity $\mathbf{D}\in\mathfrak{u}(L)$ is described by

$$\mathbf{G}_{\mathbf{I}}(\mu) = \exp(\mu\mathbf{D}), \tag{32}$$

where $\exp(\mathbf{A}) = \sum_{k=0}^{\infty}(\mathbf{A}^k/k!)$ is the matrix exponential and μ is the step size (i.e., magnitude of the tangent vector).

6) *Translate to the geodesic at $\mathbf{\Theta}_g^{(r)}$:* The geodesic emanating from $\mathbf{\Theta}_g^{(r)}$ terminates at $\mathbf{\Theta}_g^{(r+1)}$ by multiplicative updates

$$\mathbf{\Theta}_g^{(r+1)} = \mathbf{G}_{\mathbf{\Theta}_g^{(r)}}(\mu) = \mathbf{G}_{\mathbf{I}}(\mu)\mathbf{\Theta}_g^{(r)} = \exp(\mu\mathbf{D}_g^{(r)})\mathbf{\Theta}_g^{(r)}, \tag{33}$$

where μ is the step size refinable[16] by the Armijo rule [60].

Algorithm 1 summarizes the introduced group-wise geodesic RCG method. Compared to the non-geodesic approach, it leverages Lie algebra to replace the add-then-retract update with a multiplicative update (33) along the geodesics of the Stiefel manifold. This appropriate parameter space leads to faster convergence and easier step size tuning. Convergence to a local optimum is still guaranteed if not initialized at a stationary point. The group-wise updates can be performed in parallel to facilitate large-scale BD-RIS design problems. One can also directly operate on $\mathbf{\Theta}$ and pinching (i.e., keeping the main block diagonal and nulling others) relevant expressions to accelerate the algorithm for a large G.

We now analyze the computational complexity of solving singular value shaping problem (25) by Algorithm 1. To update each BD-RIS group, SVD of $\mathbf{H}$ requires $\mathcal{O}(NN_\mathrm{T}N_\mathrm{R})$, Euclidean sub-gradient (26) requires $\mathcal{O}\big(LN(N_\mathrm{T}+N_\mathrm{R}+L)\big)$, Riemannian sub-gradient translation (29) requires $\mathcal{O}(L^3)$, deviation parameter (31) and conjugate direction (30) together require $\mathcal{O}(L^2)$, and matrix exponential (33) requires $\mathcal{O}(L^3)$ operations [61]. The overall complexity is thus $\mathcal{O}\big(I_\mathrm{RCG}G(NN_\mathrm{T}N_\mathrm{R} + LN(N_\mathrm{T}+N_\mathrm{R}+L) + I_\mathrm{BLS}L^3)\big)$, where I_RCG and I_BLS are the number of iterations for geodesic RCG

[13]A geodesic is a curve representing the shortest path between two points in a Riemannian manifold, whose tangent vectors remain parallel when transporting along the curve.

[14]f is not necessarily the symmetric gauge function (25a).

[15]Lie algebra refers to the tangent space of the Lie group at the identity element. A Lie group is simultaneously a continuous group and a differentiable manifold. In this example, $\mathbb{U}^{L\times L}$ formulates a Lie group and the corresponding Lie algebra consists of skew-Hermitian matrices $\mathfrak{u}(L) \triangleq \mathcal{T}_{\mathbf{I}}\mathbb{U}^{L\times L} = \{\mathbf{M}\in\mathbb{C}^{L\times L} \mid \mathbf{M}^{\mathsf{H}}+\mathbf{M}=\mathbf{0}\}$.

[16]To double the step size, one can simply square the rotation matrix instead of recomputing the matrix exponential, that is, $\exp^2(\mu\mathbf{D}_g^{(r)}) = \exp(2\mu\mathbf{D}_g^{(r)})$.

Algorithm 1 Group-wise geodesic RCG

Input: $f(\mathbf{\Theta})$, G

Output: $\mathbf{\Theta}^{\star}$

1: **Initialize** $r \leftarrow 0$, $\mathbf{\Theta}^{(0)}$
2: **Repeat**
3: **For** $g \leftarrow 1$ to G
4: $\nabla_{\mathrm{E},g}^{(r)} \leftarrow$ (27), $\tilde{\nabla}_{\mathrm{R},g}^{(r)} \leftarrow$ (29)
5: $\tilde{\gamma}_g^{(r)} \leftarrow$ (31), $\mathbf{D}_g^{(r)} \leftarrow$ (30)
6: **If** $\Re\{\mathrm{tr}(\mathbf{D}_g^{(r)\mathsf{H}} \tilde{\nabla}_{\mathrm{R},g}^{(r)})\} < 0$ ▷ Not ascent
7: $\mathbf{D}_g^{(r)} \leftarrow \tilde{\nabla}_{\mathrm{R},g}^{(r)}$
8: **End If**
9: $\mu \leftarrow 0.1$
10: $\mathbf{G}_{\mathbf{\Theta}_g^{(r)}}(\mu) \leftarrow$ (33)
11: **While** $f\big(\mathbf{G}_{\mathbf{\Theta}_g^{(r)}}(2\mu)\big) - f(\mathbf{\Theta}_g^{(r)}) \geq \mu \cdot \frac{\mathrm{tr}(\mathbf{D}_g^{(r)} \mathbf{D}_g^{(r)\mathsf{H}})}{2}$
12: $\mu \leftarrow 2\mu$
13: **End While**
14: **While** $f\big(\mathbf{G}_{\mathbf{\Theta}_g^{(r)}}(\mu)\big) - f(\mathbf{\Theta}_g^{(r)}) < \frac{\mu}{2} \cdot \frac{\mathrm{tr}(\mathbf{D}_g^{(r)} \mathbf{D}_g^{(r)\mathsf{H}})}{2}$
15: $\mu \leftarrow \mu/2$
16: **End While**
17: $\mathbf{\Theta}_g^{(r+1)} \leftarrow$ (33)
18: **End For**
19: $r \leftarrow r+1$
20: **Until** $|f(\mathbf{\Theta}^{(r)}) - f(\mathbf{\Theta}^{(r-1)})| / f(\mathbf{\Theta}^{(r-1)}) \leq \epsilon$

and backtracking line search (i.e., line 11–16 of Algorithm 1), respectively. That is, $\mathcal{O}_{\mathrm{D}}\big(N_{\mathrm{S}}\big)$ for D-RIS and $\mathcal{O}_{\mathrm{BD}}\big(N_{\mathrm{S}}^3\big)$ for fully-connected BD-RIS.

To validate Algorithm 1 and quantify the shaping capability of BD-RIS, we characterize the achievable singular value region of BD-RIS-aided MIMO channel by considering the Pareto optimization problem

$$\max_{\mathbf{\Theta}} \quad \sum_{n=1}^{N} \rho_n \sigma_n(\mathbf{H}) \tag{34a}$$

$$\text{s.t.} \quad \mathbf{\Theta}_g^{\mathsf{H}} \mathbf{\Theta}_g = \mathbf{I}, \quad \forall g, \tag{34b}$$

where $\rho_n \geq 0$ is the weight associated with the n-th channel singular value. Varying those weights help to characterize the Pareto frontier of singular values that encloses the achievable region. While the objective (34a) does not suggest any meaningful performance metric (e.g., capacity or power gain), there exists an implicit relation since stronger channel shaping capability translates to better wireless performance. Problem (34) also generalizes the DoF problem in Proposition 1 and the individual singular value shaping problem in Corollary 3.3 and Proposition 2. It can be solved optimally by Algorithm 1 with $\mathbf{D}_{[n,n]} = \rho_n$ in (26).

IV. Rate Maximization

In this section, we first solve rate maximization problem for BD-RIS-aided MIMO point-to-point and interference channels optimally by joint beamforming design, and then exploit channel shaping for a low-complexity two-stage solution.

A. MIMO Point-to-Point Channel

The achievable rate maximization problem for BD-RIS-aided MIMO point-to-point channel is formulated as

$$\max_{\mathbf{W},\mathbf{\Theta}} \quad R = \log\det\left(\mathbf{I} + \frac{\mathbf{W}^{\mathsf{H}}\mathbf{H}^{\mathsf{H}}\mathbf{H}\mathbf{W}}{\eta}\right) \tag{35a}$$

$$\text{s.t.} \quad \|\mathbf{W}\|_{\mathrm{F}}^2 \leq P, \tag{35b}$$

$$\mathbf{\Theta}_g^{\mathsf{H}} \mathbf{\Theta}_g = \mathbf{I}, \quad \forall g, \tag{35c}$$

where $\mathbf{W}$ is the transmit precoder, R is the achievable rate, η is the average noise power, and P is maximum average transmit power. Problem (35) is non-convex due to the block-unitary constraint (35c) and the coupling between variables. Two approaches are proposed to solve it optimally or efficiently.

1) Alternating Optimization: This approach updates $\mathbf{\Theta}$ and $\mathbf{W}$ iteratively until convergence. For a given $\mathbf{W}$, the passive beamforming subproblem is

$$\max_{\mathbf{\Theta}} \quad \log\det\left(\mathbf{I} + \frac{\mathbf{H}\mathbf{Q}\mathbf{H}^{\mathsf{H}}}{\eta}\right) \tag{36a}$$

$$\text{s.t.} \quad \mathbf{\Theta}_g^{\mathsf{H}} \mathbf{\Theta}_g = \mathbf{I}, \quad \forall g, \tag{36b}$$

where $\mathbf{Q} \triangleq \mathbf{W}\mathbf{W}^{\mathsf{H}}$ is the transmit covariance matrix. Problem (36) can be solved optimally by Algorithm 1 with the partial derivative given in Lemma 1.

Lemma 1. *The partial derivative of* (36a) *with respect to BD-RIS block g is*

$$\frac{\partial R}{\partial \mathbf{\Theta}_g^*} = \frac{1}{\eta} \mathbf{H}_{\mathrm{B},g}^{\mathsf{H}} \left(\mathbf{I} + \frac{\mathbf{H}\mathbf{Q}\mathbf{H}^{\mathsf{H}}}{\eta}\right)^{-1} \mathbf{H}\mathbf{Q}\mathbf{H}_{\mathrm{F},g}^{\mathsf{H}}. \tag{37}$$

Proof. Please refer to Appendix I. □

For a given $\mathbf{\Theta}$, the optimal transmit precoder is given by eigenmode transmission [54]

$$\mathbf{W}^{\star} = \mathbf{V}\mathrm{diag}(\mathbf{s}^{\star})^{1/2}, \tag{38}$$

where $\mathbf{V}$ is the right singular matrix of $\mathbf{H}$ and $\mathbf{s}^{\star}$ is the optimal water-filling power allocation [54]. The AO algorithm is guaranteed to converge to local-optimal points of problem (35) since each subproblem is solved optimally and the objective is bounded above. The computational complexity of solving subproblem (36) by geodesic RCG is $\mathcal{O}\big(I_{\mathrm{RCG}} G (N L^2 + L N_{\mathrm{T}} N_{\mathrm{R}} + N_{\mathrm{T}}^2 N_{\mathrm{R}} + N_{\mathrm{T}} N_{\mathrm{R}}^2 + N_{\mathrm{R}}^3 + I_{\mathrm{BLS}} L^3)\big)$. On the other hand, the complexity of solving active beamforming subproblem by (38) is $\mathcal{O}\big(N N_{\mathrm{T}} N_{\mathrm{R}}\big)$. The overall complexity is thus $\mathcal{O}\big(I_{\mathrm{AO}}\big(I_{\mathrm{RCG}} G (N L^2 + L N_{\mathrm{T}} N_{\mathrm{R}} + N_{\mathrm{T}}^2 N_{\mathrm{R}} + N_{\mathrm{T}} N_{\mathrm{R}}^2 + N_{\mathrm{R}}^3 + I_{\mathrm{BLS}} L^3) + N N_{\mathrm{T}} N_{\mathrm{R}}\big)\big)$, where I_{AO} is the number of iterations for AO. That is, $\mathcal{O}_{\mathrm{D}}\big(N_{\mathrm{S}}\big)$ for D-RIS and $\mathcal{O}_{\mathrm{BD}}\big(N_{\mathrm{S}}^3\big)$ for fully-connected BD-RIS.

2) Low-Complexity Solution: To reduce the computational complexity, we suboptimally decouple the beamforming design by first shape the channel by RIS for maximum power gain and then optimize the active beamforming. The channel power gain maximization problem is formulated as[17]

$$\max_{\mathbf{\Theta}} \quad \|\mathbf{H}_{\mathrm{D}}+\mathbf{H}_{\mathrm{B}}\mathbf{\Theta}\mathbf{H}_{\mathrm{F}}\|_{\mathrm{F}}^2 \tag{39a}$$

$$\text{s.t.} \quad \mathbf{\Theta}_g^{\mathsf{H}}\mathbf{\Theta}_g=\mathbf{I}, \quad \forall g. \tag{39b}$$

Inspired by [62], we propose a closed-form iterative solution that converges to a stationary point of Problem (39). The idea is to approximate the quadratic objective (39a) successively by Taylor expansion and solve each subproblem by group-wise SVD.

Proposition 5. *Starting from any feasible $\mathbf{\Theta}^{(0)}$, the sequence*

$$\mathbf{\Theta}_g^{(r+1)}=\mathbf{U}_g^{(r)}\mathbf{V}_g^{(r)}, \quad \forall g \tag{40}$$

leads to a convergence of the objective function (39a) *towards a stationary point,*[18] *where $\mathbf{U}_g^{(r)}$ and $\mathbf{V}_g^{(r)}$ are any left and right singular matrices of*[19]

$$\mathbf{M}_g^{(r)}=\mathbf{H}_{\mathrm{B},g}^{\mathsf{H}}\Big(\mathbf{H}_{\mathrm{D}}+\mathbf{H}_{\mathrm{B}}\mathrm{diag}\big(\mathbf{\Theta}_{[1:g-1]}^{(r+1)},\mathbf{\Theta}_{[g:G]}^{(r)}\big)\mathbf{H}_{\mathrm{F}}\Big)\mathbf{H}_{\mathrm{F},g}^{\mathsf{H}}. \tag{41}$$

Proof. Please refer to Appendix J. □

To update each BD-RIS group, matrix multiplication (41) requires $\mathcal{O}\big(N_{\mathrm{T}}N_{\mathrm{R}}+NL^2+N_{\mathrm{T}}N_{\mathrm{R}}L\big)$ operations and its SVD requires $\mathcal{O}(L^3)$ operations. The overall complexity is thus $\mathcal{O}\big(I_{\mathrm{SAA}}G\big(N_{\mathrm{T}}N_{\mathrm{R}}+NL^2+N_{\mathrm{T}}N_{\mathrm{R}}L+L^3\big)\big)$, where I_{SAA} is the number iterations for successive affine approximation. That is, $\mathcal{O}_{\mathrm{D}}\big(N_{\mathrm{S}}\big)$ for D-RIS and $\mathcal{O}_{\mathrm{BD}}\big(N_{\mathrm{S}}^3\big)$ for fully-connected BD-RIS. For the latter, the computational complexity can be further reduced:

- *Negligible direct channel:* The optimal solution to (39) has been solved in closed form by (20a).
- *Non-negligible direct channel:* In terms of maximizing the inner product $\langle\mathbf{H}_{\mathrm{D}},\mathbf{H}_{\mathrm{B}}\mathbf{\Theta}\mathbf{H}_{\mathrm{F}}\rangle$, (39) is reminiscent of the weighted orthogonal Procrustes problem [63]

$$\min_{\mathbf{\Theta}} \quad \|\mathbf{H}_{\mathrm{D}}-\mathbf{H}_{\mathrm{B}}\mathbf{\Theta}\mathbf{H}_{\mathrm{F}}\|_{\mathrm{F}}^2 \tag{42a}$$

$$\text{s.t.} \quad \mathbf{\Theta}^{\mathsf{H}}\mathbf{\Theta}=\mathbf{I}, \tag{42b}$$

which still has no trivial solution. One *lossy* transformation [64] shifts $\mathbf{\Theta}$ to sides of the product by Moore-Penrose inverse, formulating standard orthogonal Procrustes problems

$$\min_{\mathbf{\Theta}} \quad \|\mathbf{H}_{\mathrm{B}}^{\dagger}\mathbf{H}_{\mathrm{D}}-\mathbf{\Theta}\mathbf{H}_{\mathrm{F}}\|_{\mathrm{F}}^2 \text{ or } \|\mathbf{H}_{\mathrm{D}}\mathbf{H}_{\mathrm{F}}^{\dagger}-\mathbf{H}_{\mathrm{B}}\mathbf{\Theta}\|_{\mathrm{F}}^2 \tag{43a}$$

$$\text{s.t.} \quad \mathbf{\Theta}^{\mathsf{H}}\mathbf{\Theta}=\mathbf{I}, \tag{43b}$$

with optimal solutions [65, (6.4.1)]

$$\mathbf{\Theta}_{\text{P-max-approx}}^{\text{MIMO-HD}}=\mathbf{U}\mathbf{V}^{\mathsf{H}}, \tag{44}$$

where $\mathbf{U}$ and $\mathbf{V}$ are respectively any left and right singular matrices of $\mathbf{H}_{\mathrm{B}}^{\dagger}\mathbf{H}_{\mathrm{D}}\mathbf{H}_{\mathrm{F}}^{\mathsf{H}}$ or $\mathbf{H}_{\mathrm{B}}^{\mathsf{H}}\mathbf{H}_{\mathrm{D}}\mathbf{H}_{\mathrm{F}}^{\dagger}$.

[17]Problem (39) has been studied in SISO [30] and MISO equivalents [31], [33], [40], [45] where only one mode is available. Generalizing those to MIMO is non-trivial due to trade-off between modes.

[18]However, (40) might not converge to a single solution point due to the non-uniqueness of SVD, especially when $\mathbf{M}_g$ is rank-deficient.

[19]We notice that the orthogonal projection of $\mathbf{M}_g$ onto the Stiefel manifold $\pi(\mathbf{M}_g)=\arg\min_{\mathbf{X}_g\in\mathbb{U}^{L\times L}}\|\mathbf{M}_g-\mathbf{X}_g\|_{\mathrm{F}}=\mathbf{U}_g\mathbf{V}_g$ coincides with $\mathbf{\Theta}_g$.

Although (20a) and (44) are of similar form, the latter is neither optimal nor a generalization of the former due to the lossy transformation. We will show in Section V that $\mathbf{\Theta}_{\text{P-max-approx}}^{\text{MIMO-HD}}$ is very close to optimal especially for a large N_{S}. Once the channel is shaped by (40) or (20a) or (44), the active beamforming is retrieved by (38). This two-stage solution avoids outer iterations and efficiently handles (or avoids) inner iterations.

B. MIMO Interference Channel

On top of (7), the achievable rate of transmission k is

$$R_k=\log\det\Big(\mathbf{I}+\mathbf{W}_k\mathbf{H}^{(kj)\mathsf{H}}\mathbf{Q}_k^{-1}\mathbf{H}^{(kj)}\mathbf{W}_k\Big), \tag{45}$$

where $\mathbf{W}_k$ is the precoder at transmitter k and $\mathbf{Q}_k=\sum_{j\neq k}\mathbf{H}^{(kj)}\mathbf{W}_j\mathbf{W}_j^{\mathsf{H}}\mathbf{H}^{(kj)\mathsf{H}}+\eta\mathbf{I}$ is the interference-plus-noise covariance matrix at receiver k. The weighted sum-rate maximization problem for BD-RIS-aided MIMO interference channel is formulated as

$$\max_{\mathbf{\Theta},\{\mathbf{W}_k\}_{k\in[K]}} \quad \sum_{k=1}^{K}\rho_k R_k \tag{46a}$$

$$\text{s.t.} \quad \mathbf{\Theta}_g^{\mathsf{H}}\mathbf{\Theta}_g=\mathbf{I}, \quad \forall g, \tag{46b}$$

$$\|\mathbf{W}_k\|_{\mathrm{F}}^2\leq P_k. \quad \forall k \tag{46c}$$

where $\rho_k\geq 0$ is the weight associated with transmission k. This non-convex problem can be solved by extending both solutions covered in Section IV-A as detailed below.

1) Alternating Optimization: This approach updates $\mathbf{\Theta}$ and $\{\mathbf{W}_k\}_{k\in[K]}$ iteratively until convergence. For a given precoder set, the passive beamforming subproblem is

$$\max_{\mathbf{\Theta}} \quad \sum_{k=1}^{K}\rho_k R_k \tag{47a}$$

$$\text{s.t.} \quad \mathbf{\Theta}_g^{\mathsf{H}}\mathbf{\Theta}_g=\mathbf{I}, \quad \forall g, \tag{47b}$$

which can be solved optimally by Algorithm 1 with the partial derivative given in Lemma 2.

Lemma 2. *The partial derivative of* (47a) *with respect to BD-RIS block g is*

$$\frac{\partial\rho_k R_k}{\partial\mathbf{\Theta}_g^*}=\sum_{k=1}^{K}\rho_k\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\mathbf{Q}_k^{-1}\mathbf{H}^{(kk)}\mathbf{W}_k\mathbf{E}_k\mathbf{W}_k^{\mathsf{H}} \times\Big(\mathbf{H}_{\mathrm{F},g}^{(k)\mathsf{H}}-\mathbf{H}^{(kk)\mathsf{H}}\mathbf{Q}_k^{-1}\sum_{j\neq k}\mathbf{H}^{(kj)}\mathbf{W}_j\mathbf{W}_j^{\mathsf{H}}\mathbf{H}_{\mathrm{F},g}^{(j)\mathsf{H}}\Big), \tag{48}$$

where $\mathbf{E}_k=\big(\mathbf{I}+\mathbf{W}_k^{\mathsf{H}}\mathbf{H}^{(kk)\mathsf{H}}\mathbf{Q}_k\mathbf{H}^{(kk)}\mathbf{W}_k\big)^{-1}$ is the error matrix of receiver k.

Proof. Please refer to Appendix K. □

For a given $\mathbf{\Theta}$, problem (46) reduces to conventional precoding design for interference channel. A closed-form iterative solution based on mutual information-Minimum Mean-Square Error (MMSE) relationship has been proposed in

[66], [67] and we summarize the steps as follows. At iteration r, the MMSE combiner at receiver k is

$$\begin{aligned}\mathbf{G}_k^{(r)} = &\mathbf{W}_k^{(r-1)\mathsf{H}}\mathbf{H}^{(kk)\mathsf{H}} \\ &\times\left(\mathbf{Q}_k^{(r-1)}+\mathbf{H}^{(kk)}\mathbf{W}_k^{(r-1)}\mathbf{W}_k^{(r-1)\mathsf{H}}\mathbf{H}^{(kk)\mathsf{H}}\right)^{-1},\end{aligned} \tag{49}$$

the corresponding error matrix is

$$\mathbf{E}_k^{(r)} = \left(\mathbf{I}+\mathbf{W}_k^{(r-1)\mathsf{H}}\mathbf{H}^{(kk)\mathsf{H}}\mathbf{Q}_k^{(r-1)}\mathbf{H}^{(kk)}\mathbf{W}_k^{(r-1)}\right)^{-1}, \tag{50}$$

and the optimal precoder at transmitter k is given by

$$\begin{aligned}\mathbf{W}_k^{(r)} = &\left(\sum_{j=1}^{K}\mathbf{H}^{(jk)\mathsf{H}}\mathbf{G}_j^{(r)\mathsf{H}}\mathbf{\Omega}_k^{(r)}\mathbf{G}_j^{(r)}\mathbf{H}^{(jk)}+\lambda_k^{(r)}\mathbf{I}\right)^{-1} \\ &\times\mathbf{H}^{(kk)\mathsf{H}}\mathbf{G}_j^{(r)\mathsf{H}}\mathbf{\Omega}_k^{(r)},\end{aligned} \tag{51}$$

where $\mathbf{\Omega}_k^{(r)} = \rho_k\mathbf{E}_k^{(r)-1}$ is the mean-square error weight and $\lambda_k^{(r)}$ is the Lagrange multiplier retrievable by bisection [66] or in closed form [67]

$$\lambda_k^{(r)} = \frac{\mathrm{tr}\left(\eta\mathbf{\Omega}_k^{(r)}\mathbf{G}_k^{(r)}\mathbf{G}_k^{(r)\mathsf{H}}+\sum_{j=1}^{K}(\mathbf{Z}_{kj}^{(r)}-\mathbf{Z}_{jk}^{(r)})\right)}{P_k}, \tag{52}$$

where $\mathbf{Z}_{kj}^{(r)} = \mathbf{\Omega}_k^{(r)}\mathbf{T}_{kj}^{(r)}\mathbf{T}_{kj}^{(r)\mathsf{H}}$ and $\mathbf{T}_{kj}^{(r)} = \mathbf{G}_k^{(r)}\mathbf{H}^{(kj)}\mathbf{W}_j^{(r)}$.

The computational complexity of solving subproblem (47) by geodesic RCG is $\mathcal{O}\big(I_{\mathrm{RCG}}G(N_{\mathrm{T}}d^2+N_{\mathrm{T}}^2d+N_{\mathrm{T}}^2N_{\mathrm{R}}+N_{\mathrm{T}}N_{\mathrm{R}}^2+K(N_{\mathrm{T}}N_{\mathrm{R}}d+N_{\mathrm{T}}N_{\mathrm{R}}L)+I_{\mathrm{BLS}}L^3)\big)$. That is, $\mathcal{O}_{\mathrm{D}}\big(N_{\mathrm{S}}\big)$ for D-RIS and $\mathcal{O}_{\mathrm{BD}}\big(N_{\mathrm{S}}^3\big)$ for fully-connected BD-RIS.

2) Low-Complexity Solution: Similar to Section IV-A2, we suboptimally decouple the beamforming design by first shape the channel by RIS for minimum leakage interference and then optimize the active beamforming. The leakage interference minimization problem is formulated as

$$\min_{\mathbf{\Theta}} \quad I = \sum_{k=1}^{K}\sum_{j\neq k}\left\|\mathbf{H}_{\mathrm{D}}^{(kj)}+\mathbf{H}_{\mathrm{B}}^{(k)}\mathbf{\Theta}\mathbf{H}_{\mathrm{F}}^{(j)}\right\|_{\mathrm{F}}^2 \tag{53a}$$

$$\text{s.t.} \quad \mathbf{\Theta}_g^{\mathsf{H}}\mathbf{\Theta}_g = \mathbf{I}, \quad \forall g, \tag{53b}$$

which can be solved iteratively in closed form.

Proposition 6. *Starting from any feasible $\mathbf{\Theta}^{(0)}$, the sequence*

$$\mathbf{\Theta}_g^{(r+1)} = \mathbf{U}_g^{(r)}\mathbf{V}_g^{(r)}, \quad \forall g \tag{54}$$

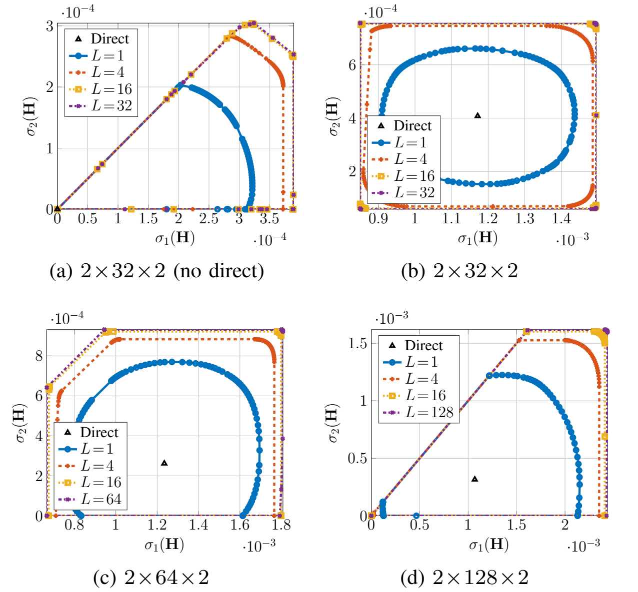
converges to a stationary point of (53)*, where $\mathbf{U}_g^{(r)}$ and $\mathbf{V}_g^{(r)}$ are any left and right singular matrices of*

$$\mathbf{M}_g^{(r)} = \sum_{k=1}^{K}\sum_{j\neq k}\left(\mathbf{B}_g^{(k)}\mathbf{\Theta}_g^{(r)}\mathbf{H}_{\mathrm{F},g}^{(j)}-\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\mathbf{D}_g^{(kj)(r)}\right)\mathbf{H}_{\mathrm{F},g}^{(j)\mathsf{H}}, \tag{55}$$

where $\mathbf{B}_g^{(k)} = \lambda_1\big(\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\mathbf{H}_{\mathrm{B},g}^{(k)}\big)\mathbf{I}-\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\mathbf{H}_{\mathrm{B},g}^{(k)}$ and $\mathbf{D}_g^{(kj)(r)} = \mathbf{H}_{\mathrm{D}}^{(kj)}+\sum_{g'<g}\mathbf{H}_{\mathrm{B},g'}^{(k)\mathsf{H}}\mathbf{\Theta}_{g'}^{(r+1)}\mathbf{H}_{\mathrm{F},g'}^{(k)}+\sum_{g'>g}\mathbf{H}_{\mathrm{B},g'}^{(k)\mathsf{H}}\mathbf{\Theta}_{g'}^{(r)}\mathbf{H}_{\mathrm{F},g'}^{(k)}$.

Proof. Please refer to Appendix L. □

Once the channel is shaped by (54), the active beamforming is retrieved iteratively by (51). This Two-stage solution avoids outer iterations and efficiently handles inner iterations.



(a) $2\times32\times2$ (no direct)

(b) $2\times32\times2$

(c) $2\times64\times2$

(d) $2\times128\times2$

Fig. 2. Pareto frontiers of singular values of an $N_{\mathrm{T}} = N_{\mathrm{R}} = 2$ channel reshaped by BD-RIS.

V. Simulation Results

In this section, we provide numerical results to evaluate the proposed BD-RIS designs.[20] Consider a distance-dependent path loss model $\Lambda(d) = \Lambda_0 d^{-\gamma}$ where Λ_0 is the reference path loss at distance $1\,\mathrm{m}$, d is the propagation distance, and γ is the path loss exponent. The small-scale fading model is $\mathbf{H} = \sqrt{\kappa/(1+\kappa)}\mathbf{H}_{\mathrm{LoS}}+\sqrt{1/(1+\kappa)}\mathbf{H}_{\mathrm{NLoS}}$, where κ is the Rician K-factor, $\mathbf{H}_{\mathrm{LoS}}$ is the deterministic LoS component, and $\mathbf{H}_{\mathrm{NLoS}} \sim \mathcal{N}_{\mathbb{C}}(\mathbf{0},\mathbf{I})$ is the Rayleigh component. We set $\Lambda_0 = -30\,\mathrm{dB}$, $d_{\mathrm{D}} = 14.7\mathrm{m}$, $d_{\mathrm{F}} = 10\mathrm{m}$, $d_{\mathrm{B}} = 6.3\mathrm{m}$, $\gamma_{\mathrm{D}} = 3$, $\gamma_{\mathrm{F}} = 2.4$ and $\gamma_{\mathrm{B}} = 2$ for reference, which corresponds to a typical indoor environment with $\Lambda_{\mathrm{D}} = -65\mathrm{dB}$, $\Lambda_{\mathrm{F}} = -54\mathrm{dB}$, $\Lambda_{\mathrm{B}} = -46\mathrm{dB}$. The indirect path via RIS is thus $35\,\mathrm{dB}$ weaker than the direct path. Rayleigh fading (i.e., $\kappa = 0$) is assumed for all channels unless otherwise specified.

A. Algorithm Evaluation

We first compare in Table I the geodesic and non-geodesic RCG algorithm on problem (34) in an $N_{\mathrm{T}} = N_{\mathrm{R}} = 4$ system with BD-RIS group size $L = 4$. The statistics are averaged over 100 independent runs. It is observed that the geodesic RCG method achieves a slightly higher objective value with significantly (down to 1/3) lower number of iterations and shorter (down to 1/4) computational time than the non-geodesic method. The results demonstrate the efficiency of the proposed geodesic RCG algorithm especially for large-scale BD-RIS design problems.

B. Channel Singular Values Redistribution

1) Pareto Frontier: Fig. 2 shows the Pareto singular values of an $N_{\mathrm{T}} = N_{\mathrm{R}} = 2$ MIMO reshaped by a RIS. When the direct channel is negligible, the achievable regions in Fig. 2(a) are

[20] Source code is available at https://github.com/snowztail/channel-shaping.

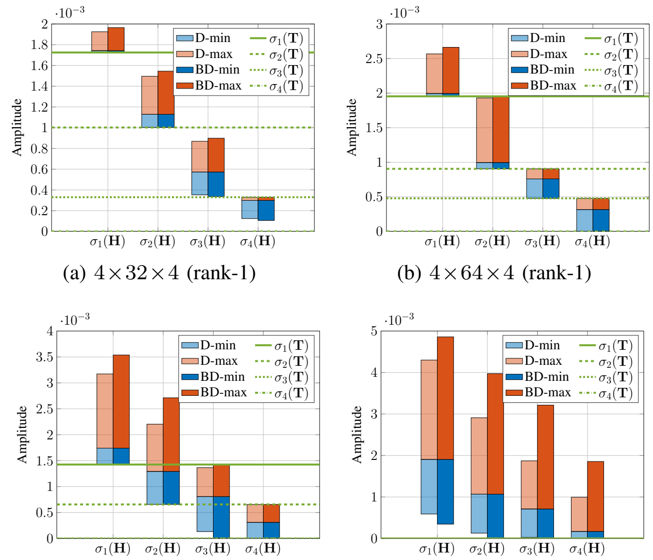
TABLE I
AVERAGE PERFORMANCE OF GEODESIC AND NON-GEODESIC RCG ALGORITHMS ON PROBLEM (34)

RCG path	$N_\mathrm{S}=16$			$N_\mathrm{S}=256$		
	Objective	Iterations	Time [s]	Objective	Iterations	Time [s]
Geodesic	4.359×10^{-3}	11.59	1.839×10^{-2}	1.163×10^{-2}	25.58	3.461
Non-geodesic	4.329×10^{-3}	30.92	5.743×10^{-2}	1.116×10^{-2}	61.40	13.50

shaped like pizza slices. This is because $\sigma_1(\mathbf{H})\geq\sigma_2(\mathbf{H})\geq0$ and there exists a trade-off between the alignment of two spaces. We observe that the smallest singular value can be enhanced up to 2×10^{-4} by D-RIS and 3×10^{-4} by fully-connected BD-RIS, corresponding to a $50\,\%$ gain. When the direct channel is significant, the shape of the singular value region depends heavily on the relative strength of the indirect channels. In Fig. 2(b), a 32-element RIS is insufficient to compensate the $35\,\mathrm{dB}$ path loss imbalance and results in a limited singular value region that is symmetric around the direct point. As the group size L increases, the shape of the region evolves from elliptical to square. This transformation not only improves the dynamic range of $\sigma_1(\mathbf{H})$ and $\sigma_2(\mathbf{H})$ by $22\,\%$ and $38\,\%$, but also provides a better trade-off in manipulating both singular values. It suggests the design flexibility from larger group size allows better alignment of multiple singular vector spaces simultaneously. The singular value region also enlarges as the number of scattering elements N_S increases. In particular, Fig. 2(d) shows that the equivalent channel can be completely nulled (corresponding to the origin) by a 128-element BD-RIS thanks to its superior channel shaping capability, but not by a diagonal one. Those results demonstrate the superior channel shaping capability of BD-RIS and emphasizes the importance of reconfigurable inter-connections between elements.

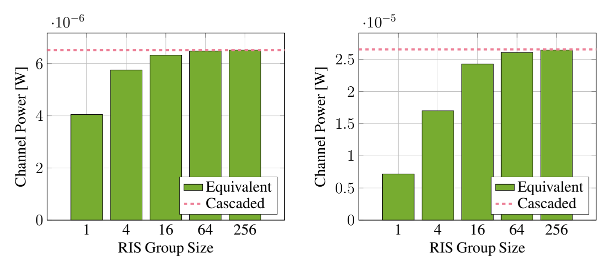
2) Analytical Bounds and Numerical Results: Fig. 3 illustrates the analytical singular value bounds in Proposition 2 and the numerical results obtained by solving problem (34). Here we consider a rank-k forward channel without loss of generality. When the RIS is in the vicinity of the transmitter, Figs. 3(a) and 3(b) show that the achievable channel singular values indeed satisfy Corollary 2.1, namely $\sigma_1(\mathbf{H})\geq\sigma_1(\mathbf{T})$, $\sigma_2(\mathbf{T})\leq\sigma_2(\mathbf{H})\leq\sigma_1(\mathbf{T})$, etc. It is obvious that BD-RIS can approach those bounds better than D-RIS especially for a small N_S. Another example is given in Fig. 3(c) with rank-2 forward channel. The first two channel singular values are unbounded above and bounded below by the first two singular values of $\mathbf{T}$, while the last two singular values can be suppressed to zero and bounded above by the first two singular values of $\mathbf{T}$. Those observations align with Proposition 2. Finally, Fig. 3(d) confirms there are no extra singular value bounds when both backward and forward channels are full-rank. This can be predicted from (9) where the singular matrix $\mathbf{V}_\mathrm{F}$ becomes unitary and $\mathbf{T}=\mathbf{0}$. The numerical results are consistent with the analytical bounds, and we conclude that the channel shaping advantage of BD-RIS over D-RIS scales with backward and forward channel ranks.

Fig. 4 compares the analytical channel power bound in Corollary 3.4 and the numerical results obtained by solving problem (39) when the direct channel is negligible. Here, a fully-connected BD-RIS can attain the upper bound either in closed form (20a) or via optimization approach (40). For the SISO case in Fig. 4(a), the maximum channel power gain is approximately 4×10^{-6} by D-RIS and 6.5×10^{-6} by fully-connected BD-RIS, corresponding to a $62.5\,\%$ gain. It comes purely from branch matching and agrees with the asymptotic power scaling law derived for SISO in [30, (30)]. Interestingly, this relative power gain surges to $270\,\%$ in $N_\mathrm{T}=N_\mathrm{R}=4$ MIMO as shown in Fig. 4(b), which can also be predicted from the expectation analysis (21). We thus conclude that the



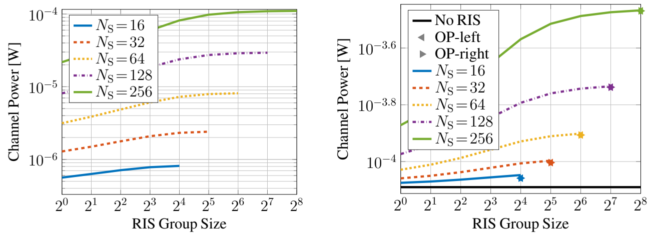
(a) $4\times32\times4$ (rank-1)
(b) $4\times64\times4$ (rank-1)
(c) $4\times128\times4$ (rank-2)
(d) $4\times256\times4$ (rank-4)

Fig. 3. Achievable channel singular values: analytical bounds (lines) and numerical results (bars). Baselines of bars denote the singular values of the direct channel. Blue (resp. red) bars denote the lower (resp. upper) dynamic range of singular values obtained by solving (34) with $\rho_n/\rho_{n'}\to0$ (resp. $\to\infty$), $\forall n,\ n'\neq n$. 'D' means D-RIS and 'BD' refers to fully-connected BD-RIS. 'rank-k' refers to the rank of the forward channel.



(a) $1\times256\times1$ (no direct)
(b) $4\times256\times4$ (no direct)

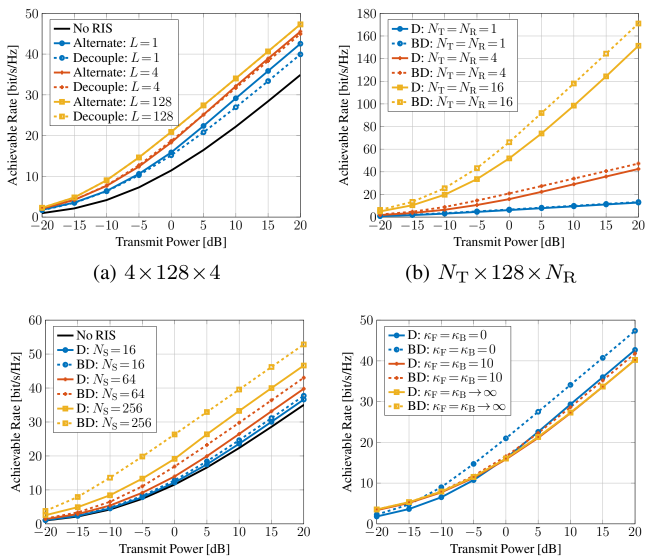
Fig. 4. Average maximum channel power gain versus BD-RIS group size and MIMO dimensions. The direct channel is negligible. 'Cascaded' refers to the available power of the cascaded channel, i.e., the sum of (sorted) element-wise power product of backward and forward channels.



(a) $16 \times N_S \times 16$ (no direct)

(b) $16 \times N_S \times 16$

Fig. 5. Average maximum channel power gain versus RIS configuration. 'OP-left' and 'OP-right' refer to the suboptimal solutions to problem (39) by lossy transformation (43) where $\boldsymbol{\Theta}$ is to the left and right of the product, respectively.



(a) $4 \times 128 \times 4$

(b) $N_T \times 128 \times N_R$

(c) $4 \times N_S \times 4$

(d) $4 \times 128 \times 4$

Fig. 6. Average achievable rate versus MIMO and RIS configurations. The noise power is $\eta = -75$dB, corresponding to a direct SNR of -10 to 30 dB. 'Alternate' refers to the alternating optimization and 'Decouple' refers to the low-complexity design. 'D' means D-RIS and 'BD' refers to fully-connected BD-RIS.

power gain of BD-RIS scales with group size and MIMO dimensions.

C. Power Gain and Achievable Rate Maximization

We first focus on channel power gain maximization problem (39). Fig. 5 shows the maximum channel power under different RIS configurations. An interesting observation is that the relative power gain of BD-RIS over D-RIS is even larger when the direct channel is significant. For example, a 64-element fully BD-RIS can almost provide the same channel power gain as a 256-element D-RIS in Fig. 5(b), but not in Fig. 5(a). This is because the RIS needs to balance the multiplicative forward-backward combining and the additive direct-indirect combining, such that the mode alignment advantage of BD-RIS becomes more pronounced. We also notice that the suboptimal solutions (44) for fully-connected BD-RIS by lossy transformation (43) are very close to optimal especially for a large N_S.

Fig. 6 presents the achievable rate under different MIMO and RIS configurations. At a transmit power $P = 10$dB, Fig. 6(a) shows that introducing a 128-element D-RIS to $N_T = N_R = 4$ MIMO can improve the achievable rate from 22.2 bps/Hz to 29.2 bps/Hz (+31.5%). A BD-RIS of group size 4 and 128 can further elevate those to 32.1 bps/Hz (+44.6%) and 34 bps/Hz (+53.2%), respectively. An interesting observation is that the rate gap between the optimal AO approach (36)–(**??**) and the shaping-inspired solution (40), (**??**) narrows at larger group size and completely vanishes for a fully-connected BD-RIS. This implies that joint RIS-transceiver designs can be decoupled by first shaping the wireless channel and then optimizing the active beamformer, which significantly simplifies the process at marginal performance cost. Figs. 6(b) and 6(c) also show that both *absolute and relative* rate gains of BD-RIS versus D-RIS increases with the number of transmit and receive antennas and scattering elements, especially at high SNR. For $N_S = 128$ and $P = 20$dB, the achievable rate ratio of BD-RIS over D-RIS is 1.04, 1.11, and 1.13 for $N_T = N_R = 1$, 4, and 16, respectively. For $N_T = N_R = 4$ and $P = 20$dB, this ratio amounts to 1.03, 1.08, and 1.13 for $N_S = 16$, 64, and 256, respectively. Those observations align with the power gain results in Fig. 5 and highlight the rate benefits of BD-RIS over D-RIS in large-scale MIMO systems. In the low power regime (-20 to -10 dB), we also notice that the slope of the achievable rate of BD-RIS is steeper than that of D-RIS. That is, BD-RIS can help to activate more streams and achieve the asymptotic DoF at a low transmit SNR. This is particularly visible in Fig. 6(c) where the topmost curve is almost a linear function of the transmit power. It is expected from the shaping results in Fig. 2 that BD-RIS can significantly enlarge all channel singular values for higher receive SNR. Finally, Fig. 6(d) shows that the gap between D- and BD-RIS narrows as the Rician K-factor increases and becomes indistinguishable in LoS environment. The observation is expected from previous studies [30], [31], [56] and aligns with Corollary 2.1, which suggests that the BD-RIS should be deployed in rich-scattering environments to exploit its channel shaping potential.

VI. Conclusion

This paper analyzes the channel shaping capability of RIS in terms of singular values redistribution. We consider a general BD architecture that allows elements within the same group to interact, enabling more sophisticated manipulation than D-RIS. This translates to a wider dynamic range of and better trade-off between singular values and significant power and rate gains, especially in large-scale MIMO systems. We characterize the Pareto frontiers of channel singular values via optimization approach and provide analytical bounds for practical deployment scenarios. Specifically, the former is done by proposing an efficient RCG algorithm for BD-RIS optimization problems, which converges much faster than existing methods. We also present two beamforming designs for rate maximization problem, one for optimal performance and the other exploits channel shaping for lower complexity. Extensive simulations show that the shaping advantage of BD-RIS stems from its superior branch matching and mode alignment potentials, which scales with the number of elements, group size, and MIMO dimensions.

Appendix

A. Proof of Proposition 1

It suffices to consider the rank of the indirect channel. Denote the SVD of the backward and forward channels as

$$\mathbf{H}_{\mathrm{B/F}} = \begin{bmatrix}\mathbf{U}_{\mathrm{B/F},1} & \mathbf{U}_{\mathrm{B/F},2}\end{bmatrix} \begin{bmatrix}\mathbf{\Sigma}_{\mathrm{B/F},1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0}\end{bmatrix} \begin{bmatrix}\mathbf{V}_{\mathrm{B/F},1}^{\mathsf{H}} \\ \mathbf{V}_{\mathrm{B/F},2}^{\mathsf{H}}\end{bmatrix},$$

where $\mathbf{U}_{\mathrm{B/F},1}$ and $\mathbf{V}_{\mathrm{B/F},1}$ are any left and right singular matrices of $\mathbf{H}_{\mathrm{B/F}}$ corresponding to non-zero singular values $\mathbf{\Sigma}_{\mathrm{B/F},1}$, and $\mathbf{U}_{\mathrm{B/F},2}$ and $\mathbf{V}_{\mathrm{B/F},2}$ are those corresponding to zero singular values. The rank of the indirect channel is [48, (16.5.10.b)]

$$\begin{aligned}\mathrm{rank}(\mathbf{H}_{\mathrm{B}}\mathbf{\Theta}\mathbf{H}_{\mathrm{F}}) &= \mathrm{rank}(\mathbf{H}_{\mathrm{B}}) - \dim\big(\ker(\mathbf{H}_{\mathrm{F}}^{\mathsf{H}}\mathbf{\Theta}^{\mathsf{H}}) \cap \mathrm{ran}(\mathbf{H}_{\mathrm{B}}^{\mathsf{H}})\big) \\ &= \mathrm{rank}(\mathbf{H}_{\mathrm{B}}) - \dim\big(\mathrm{ran}(\mathbf{\Theta}\mathbf{U}_{\mathrm{F},2}) \cap \mathrm{ran}(\mathbf{V}_{\mathrm{B},1})\big) \\ &\triangleq r_{\mathrm{B}} - r_{\mathrm{L}}(\mathbf{\Theta}),\end{aligned}$$

where we define $r_{\mathrm{L}}(\mathbf{\Theta}) \triangleq \dim\big(\mathrm{ran}(\mathbf{\Theta}\mathbf{U}_{\mathrm{F},2}) \cap \mathrm{ran}(\mathbf{V}_{\mathrm{B},1})\big)$ and $r_{\mathrm{B/F}} \triangleq \mathrm{rank}(\mathbf{H}_{\mathrm{B/F}})$. Since $\mathbf{U}_{\mathrm{F},2} \in \mathbb{U}^{N_{\mathrm{S}} \times (N_{\mathrm{S}} - r_{\mathrm{F}})}$ and $\mathbf{V}_{\mathrm{B},1} \in \mathbb{U}^{N_{\mathrm{S}} \times r_{\mathrm{B}}}$, we have $\max(r_{\mathrm{B}} - r_{\mathrm{F}}, 0) \leq r_{\mathrm{L}}(\mathbf{\Theta}) \leq \min(N_{\mathrm{S}} - r_{\mathrm{F}}, r_{\mathrm{B}})$ and thus

$$\max(r_{\mathrm{B}} + r_{\mathrm{F}} - N_{\mathrm{S}}, 0) \leq \mathrm{rank}(\mathbf{H}_{\mathrm{B}}\mathbf{\Theta}\mathbf{H}_{\mathrm{F}}) \leq \min(r_{\mathrm{B}}, r_{\mathrm{F}}). \tag{56}$$

To attain the upper bound in (56), the RIS needs to minimize $r_{\mathrm{L}}(\mathbf{\Theta})$ by aligning the ranges of $\mathbf{\Theta}\mathbf{U}_{\mathrm{F},2}$ and $\mathbf{V}_{\mathrm{B},2}$ as much as possible. This is achieved by

$$\mathbf{\Theta}_{\text{DoF-max}}^{\text{MIMO}} = \mathbf{Q}_{\mathrm{B},2}\mathbf{Q}_{\mathrm{F},2}^{\mathsf{H}}, \tag{57}$$

where $\mathbf{Q}_{\mathrm{B},2}$ and $\mathbf{Q}_{\mathrm{F},2}$ are the unitary matrices of the QR decomposition of $\mathbf{V}_{\mathrm{B},2}$ and $\mathbf{U}_{\mathrm{F},2}$, respectively. Similarly, the lower bound in (56) is attained at

$$\mathbf{\Theta}_{\text{DoF-min}}^{\text{MIMO}} = \mathbf{Q}_{\mathrm{B},1}\mathbf{Q}_{\mathrm{F},2}^{\mathsf{H}}, \tag{58}$$

where $\mathbf{Q}_{\mathrm{B},1}$ is the unitary matrix of the QR decomposition of $\mathbf{V}_{\mathrm{B},1}$. While the DoF-optimal structures (57) and (58) are always feasible for fully-connected BD-RIS, they are generally infeasible for D-RIS unless there exist some QR decomposition that diagonalize $\mathbf{Q}_{\mathrm{B},2}\mathbf{Q}_{\mathrm{F},2}^{\mathsf{H}}$ and $\mathbf{Q}_{\mathrm{B},1}\mathbf{Q}_{\mathrm{F},2}^{\mathsf{H}}$ simultaneously. That is, BD-RIS may achieve a larger or smaller number of DoF of indirect channel, and thus equivalent channel, than D-RIS.

B. Proof of Proposition 2

We consider rank-k forward channel and the proof follows similarly for rank-k backward channel. Let $\mathbf{H}_{\mathrm{F}} = \mathbf{U}_{\mathrm{F}}\mathbf{\Sigma}_{\mathrm{F}}\mathbf{V}_{\mathrm{F}}^{\mathsf{H}}$ be the SVD of the forward channel. The channel Gram matrix $\mathbf{G} \triangleq \mathbf{H}\mathbf{H}^{\mathsf{H}}$ can be written as

$$\begin{aligned}\mathbf{G} &= \mathbf{H}_{\mathrm{D}}\mathbf{H}_{\mathrm{D}}^{\mathsf{H}} + \mathbf{H}_{\mathrm{B}}\mathbf{\Theta}\mathbf{U}_{\mathrm{F}}\mathbf{\Sigma}_{\mathrm{F}}\mathbf{\Sigma}_{\mathrm{F}}^{\mathsf{H}}\mathbf{U}_{\mathrm{F}}^{\mathsf{H}}\mathbf{\Theta}^{\mathsf{H}}\mathbf{H}_{\mathrm{B}}^{\mathsf{H}} \\ &\quad + \mathbf{H}_{\mathrm{B}}\mathbf{\Theta}\mathbf{U}_{\mathrm{F}}\mathbf{\Sigma}_{\mathrm{F}}\mathbf{V}_{\mathrm{F}}^{\mathsf{H}}\mathbf{H}_{\mathrm{D}}^{\mathsf{H}} + \mathbf{H}_{\mathrm{D}}\mathbf{V}_{\mathrm{F}}\mathbf{\Sigma}_{\mathrm{F}}\mathbf{U}_{\mathrm{F}}^{\mathsf{H}}\mathbf{\Theta}^{\mathsf{H}}\mathbf{H}_{\mathrm{B}}^{\mathsf{H}} \\ &= \mathbf{H}_{\mathrm{D}}(\mathbf{I} - \mathbf{V}_{\mathrm{F}}\mathbf{V}_{\mathrm{F}}^{\mathsf{H}})\mathbf{H}_{\mathrm{D}}^{\mathsf{H}} \\ &\quad + (\mathbf{H}_{\mathrm{B}}\mathbf{\Theta}\mathbf{U}_{\mathrm{F}}\mathbf{\Sigma}_{\mathrm{F}} + \mathbf{H}_{\mathrm{D}}\mathbf{V}_{\mathrm{F}})(\mathbf{\Sigma}_{\mathrm{F}}\mathbf{U}_{\mathrm{F}}^{\mathsf{H}}\mathbf{\Theta}^{\mathsf{H}}\mathbf{H}_{\mathrm{B}}^{\mathsf{H}} + \mathbf{V}_{\mathrm{F}}^{\mathsf{H}}\mathbf{H}_{\mathrm{D}}^{\mathsf{H}}) \\ &= \mathbf{Y} + \mathbf{Z}\mathbf{Z}^{\mathsf{H}},\end{aligned}$$

where we define $\mathbf{Y} \triangleq \mathbf{H}_{\mathrm{D}}(\mathbf{I} - \mathbf{V}_{\mathrm{F}}\mathbf{V}_{\mathrm{F}}^{\mathsf{H}})\mathbf{H}_{\mathrm{D}}^{\mathsf{H}} \in \mathbb{H}^{N_{\mathrm{R}} \times N_{\mathrm{R}}}$ and $\mathbf{Z} \triangleq \mathbf{H}_{\mathrm{B}}\mathbf{\Theta}\mathbf{U}_{\mathrm{F}}\mathbf{\Sigma}_{\mathrm{F}} + \mathbf{H}_{\mathrm{D}}\mathbf{V}_{\mathrm{F}} \in \mathbb{C}^{N_{\mathrm{R}} \times k}$. That is to say, $\mathbf{G}$ can be expressed as a Hermitian matrix plus k rank-1 perturbations. According to the Cauchy interlacing formula [65, Theorem 8.4.3], the n-th eigenvalue of $\mathbf{G}$ is bounded by

$$\lambda_n(\mathbf{G}) \leq \lambda_{n-k}(\mathbf{Y}), \qquad \text{if } n > k, \tag{59}$$

$$\lambda_n(\mathbf{G}) \geq \lambda_n(\mathbf{Y}), \qquad \text{if } n < N - k + 1. \tag{60}$$

Since $\mathbf{Y} = \mathbf{T}\mathbf{T}^{\mathsf{H}}$ is positive semi-definite, taking the square roots of (59) and (60) gives (8a) and (8b).

C. Proof of Proposition 3

Let $\mathbf{H}_{\mathrm{B}} = \mathbf{U}_{\mathrm{B}}\mathbf{\Sigma}_{\mathrm{B}}\mathbf{V}_{\mathrm{B}}^{\mathsf{H}}$ and $\mathbf{H}_{\mathrm{F}} = \mathbf{U}_{\mathrm{F}}\mathbf{\Sigma}_{\mathrm{F}}\mathbf{V}_{\mathrm{F}}^{\mathsf{H}}$ be the SVD of the backward and forward channels, respectively. The scattering matrix of fully-connected BD-RIS can be decomposed as

$$\mathbf{\Theta} = \mathbf{V}_{\mathrm{B}}\mathbf{X}\mathbf{U}_{\mathrm{F}}^{\mathsf{H}}, \tag{61}$$

where $\mathbf{X} \in \mathbb{U}^{N_{\mathrm{S}} \times N_{\mathrm{S}}}$ is a unitary matrix to be designed. The equivalent channel is thus a function of $\mathbf{X}$

$$\mathbf{H} = \mathbf{H}_{\mathrm{B}}\mathbf{\Theta}\mathbf{H}_{\mathrm{F}} = \mathbf{U}_{\mathrm{B}}\mathbf{\Sigma}_{\mathrm{B}}\mathbf{X}\mathbf{\Sigma}_{\mathrm{F}}\mathbf{V}_{\mathrm{F}}^{\mathsf{H}}. \tag{62}$$

Since $\mathrm{sv}(\mathbf{U}\mathbf{A}\mathbf{V}^{\mathsf{H}}) = \mathrm{sv}(\mathbf{A})$ for unitary $\mathbf{U}$ and $\mathbf{V}$, we have

$$\begin{aligned}\mathrm{sv}(\mathbf{H}) &= \mathrm{sv}(\mathbf{U}_{\mathrm{B}}\mathbf{\Sigma}_{\mathrm{B}}\mathbf{X}\mathbf{\Sigma}_{\mathrm{F}}\mathbf{V}_{\mathrm{F}}^{\mathsf{H}}) \\ &= \mathrm{sv}(\mathbf{\Sigma}_{\mathrm{B}}\mathbf{X}\mathbf{\Sigma}_{\mathrm{F}}) \\ &= \mathrm{sv}(\bar{\mathbf{U}}_{\mathrm{B}}\mathbf{\Sigma}_{\mathrm{B}}\bar{\mathbf{V}}_{\mathrm{B}}^{\mathsf{H}}\bar{\mathbf{U}}_{\mathrm{F}}\mathbf{\Sigma}_{\mathrm{F}}\bar{\mathbf{V}}_{\mathrm{F}}^{\mathsf{H}}) \\ &= \mathrm{sv}(\mathbf{B}\mathbf{F}),\end{aligned} \tag{63}$$

where $\bar{\mathbf{U}}_{\mathrm{B}} \in \mathbb{U}^{N_{\mathrm{R}} \times N_{\mathrm{R}}}$, $\bar{\mathbf{V}}_{\mathrm{B}}, \bar{\mathbf{U}}_{\mathrm{F}} \in \mathbb{U}^{N_{\mathrm{S}} \times N_{\mathrm{S}}}$, and $\bar{\mathbf{V}}_{\mathrm{F}} \in \mathbb{U}^{N_{\mathrm{T}} \times N_{\mathrm{T}}}$ can be designed arbitrarily.

D. Proof of Corollary 3.2

(13a) follows from (12) when $r = k$. On the other hand, if we can prove

$$\prod_{n=1}^{\bar{N}} \sigma_n(\mathbf{H}) = \prod_{n=1}^{\bar{N}} \sigma_n(\mathbf{H}_{\mathrm{B}})\sigma_n(\mathbf{H}_{\mathrm{F}}), \tag{64}$$

then (13b) follows from (13a) and the non-negativity of singular values. To see (64), we start from a stricter result

$$\prod_{n=1}^{N_{\mathrm{S}}} \sigma_n(\mathbf{H}) = \prod_{n=1}^{N_{\mathrm{S}}} \sigma_n(\mathbf{H}_{\mathrm{B}})\sigma_n(\mathbf{H}_{\mathrm{F}}), \tag{65}$$

which is provable by cases. When $N_{\mathrm{S}} > N$, both sides of (65) become zero since $\sigma_n(\mathbf{H}) = \sigma_n(\mathbf{H}_{\mathrm{B}}) = \sigma_n(\mathbf{H}_{\mathrm{F}}) = 0$ for $n > N$. When $N_{\mathrm{S}} \leq N$, we have

$$\begin{aligned}\prod\nolimits_{n=1}^{N_{\mathrm{S}}} \sigma_n(\mathbf{H}) &= \prod\nolimits_{n=1}^{N_{\mathrm{S}}} \sigma_n(\mathbf{\Sigma}_{\mathrm{B}}\mathbf{X}\mathbf{\Sigma}_{\mathrm{F}}) \\ &= \prod\nolimits_{n=1}^{N_{\mathrm{S}}} \sigma_n(\hat{\mathbf{\Sigma}}_{\mathrm{B}}\mathbf{X}\hat{\mathbf{\Sigma}}_{\mathrm{F}}) \\ &= \det\big(\hat{\mathbf{\Sigma}}_{\mathrm{B}}\mathbf{X}\hat{\mathbf{\Sigma}}_{\mathrm{F}}\big) \\ &= \det\big(\hat{\mathbf{\Sigma}}_{\mathrm{B}}\big)\det(\mathbf{X})\det\big(\hat{\mathbf{\Sigma}}_{\mathrm{F}}\big) \\ &= \prod\nolimits_{n=1}^{N_{\mathrm{S}}} \sigma_n(\mathbf{\Sigma}_{\mathrm{B}})\sigma_n(\mathbf{\Sigma}_{\mathrm{F}}),\end{aligned}$$

where the first equality follows from (63) and $\hat{\mathbf{\Sigma}}_{\mathrm{B}}, \hat{\mathbf{\Sigma}}_{\mathrm{F}}$ truncate $\mathbf{\Sigma}_{\mathrm{B}}, \mathbf{\Sigma}_{\mathrm{F}}$ to square matrices of dimension N_{S}, respectively. It is evident that (65) implies (64) and thus (13b).

E. Proof of Corollary 3.3

In (14), the set of upper bounds

$$\left\{\sigma_n(\mathbf{H}) \leq \sigma_i(\mathbf{H}_\mathrm{B})\sigma_j(\mathbf{H}_\mathrm{F}) \,|\, [i,j,k] \in [N_\mathrm{S}]^3, i+j=n+1\right\} \quad (66)$$

is a special case of (12) with $(I,J,K) \in [N_\mathrm{S}]^3$. The minimum[21] of (66) is selected as the tightest upper bound in (14). On the other hand, the set of lower bounds

$$\left\{\sigma_n(\mathbf{H}) \geq \sigma_i(\mathbf{H}_\mathrm{B})\sigma_j(\mathbf{H}_\mathrm{F}) \,|\, [i,j,k] \in [N_\mathrm{S}]^3, i+j=n+N_\mathrm{S}\right\} \quad (67)$$

can be induced by (66), (65), and the non-negativity of singular values. The maximum of (67) is selected as the tightest lower bound in (14). Interested readers are also referred to [68, (2.0.3)].

To attain the upper bound, the BD-RIS needs to maximize the minimum of the first n channel singular values. It follows from (15a) that

$$\begin{aligned}\mathrm{sv}(\mathbf{H}) &= \mathrm{sv}(\mathbf{H}_\mathrm{B}\mathbf{V}_\mathrm{B}\mathbf{P}\mathbf{U}_\mathrm{F}^\mathsf{H}\mathbf{H}_\mathrm{F}) \\ &= \mathrm{sv}(\mathbf{U}_\mathrm{B}\mathbf{\Sigma}_\mathrm{B}\mathbf{V}_\mathrm{B}^\mathsf{H}\mathbf{V}_\mathrm{B}\mathbf{P}\mathbf{U}_\mathrm{F}^\mathsf{H}\mathbf{U}_\mathrm{F}\mathbf{\Sigma}_\mathrm{F}\mathbf{U}_\mathrm{F}^\mathsf{H}) \\ &= \mathrm{sv}(\mathbf{\Sigma}_\mathrm{B}\mathbf{P}\mathbf{\Sigma}_\mathrm{F}).\end{aligned}$$

On the one hand, $\mathbf{P}_{ij}=1$ with (i,j) satisfying (16a) ensures $\min_{i+j=n+1} \sigma_i(\mathbf{H}_\mathrm{B})\sigma_j(\mathbf{H}_\mathrm{F})$ is a singular value of $\mathbf{H}$. It is actually among the first n since the number of pairs (i',j') not majorized by (i,j) is $n-1$. On the other hand, (17a) ensures the first $(n-1)$-th singular values are no smaller than $\min_{i+j=n+1}\sigma_i(\mathbf{H}_\mathrm{B})\sigma_j(\mathbf{H}_\mathrm{F})$. Combining both facts, we claim the upper bound $\sigma_n(\mathbf{H}) = \min_{i+j=n+1}\sigma_i(\mathbf{H}_\mathrm{B})\sigma_j(\mathbf{H}_\mathrm{F})$ is attainable by (15a). The attainability of the lower bound can be proved similarly and the details are omitted.

F. Proof of Corollary 3.4

From (61) and (62) we have

$$\begin{aligned}\|\mathbf{H}\|_\mathrm{F}^2 &= \mathrm{tr}\left(\mathbf{V}_\mathrm{F}\mathbf{\Sigma}_\mathrm{F}^\mathsf{H}\mathbf{X}^\mathsf{H}\mathbf{\Sigma}_\mathrm{B}^\mathsf{H}\mathbf{U}_\mathrm{B}^\mathsf{H}\mathbf{U}_\mathrm{B}\mathbf{\Sigma}_\mathrm{B}\mathbf{X}\mathbf{\Sigma}_\mathrm{F}\mathbf{V}_\mathrm{F}^\mathsf{H}\right) \\ &= \mathrm{tr}\left(\mathbf{\Sigma}_\mathrm{B}^\mathsf{H}\mathbf{\Sigma}_\mathrm{B} \cdot \mathbf{X}\mathbf{\Sigma}_\mathrm{F}\mathbf{\Sigma}_\mathrm{F}^\mathsf{H}\mathbf{X}^\mathsf{H}\right) \\ &\triangleq \mathrm{tr}\left(\tilde{\mathbf{B}}\tilde{\mathbf{F}}\right),\end{aligned} \quad (68)$$

where $\mathbf{X} \triangleq \mathbf{V}_\mathrm{B}^\mathsf{H}\mathbf{\Theta}\mathbf{U}_\mathrm{F} \in \mathbb{U}^{N_\mathrm{S}\times N_\mathrm{S}}$, $\tilde{\mathbf{B}} \triangleq \mathbf{\Sigma}_\mathrm{B}^\mathsf{H}\mathbf{\Sigma}_\mathrm{B} \in \mathbb{H}_+^{N_\mathrm{S}\times N_\mathrm{S}}$, and $\tilde{\mathbf{F}} \triangleq \mathbf{X}\mathbf{\Sigma}_\mathrm{F}\mathbf{\Sigma}_\mathrm{F}^\mathsf{H}\mathbf{X}^\mathsf{H} \in \mathbb{H}_+^{N_\mathrm{S}\times N_\mathrm{S}}$. By Ruhe's trace inequality for positive semi-definite matrices [69, (H.1.g) and (H.1.h)],

$$\sum_{n=1}^{N}\lambda_n(\tilde{\mathbf{B}})\lambda_{N_\mathrm{S}-n+1}(\tilde{\mathbf{F}}) \leq \mathrm{tr}\left(\tilde{\mathbf{B}}\tilde{\mathbf{F}}\right) \leq \sum_{n=1}^{N}\lambda_n(\tilde{\mathbf{B}})\lambda_n(\tilde{\mathbf{F}}),$$

which simplifies to (19). The upper bound is attained when $\mathbf{X}$ is chosen to match the singular values of $\tilde{\mathbf{F}}$ to those of $\tilde{\mathbf{B}}$ in similar order. Apparently this occurs at $\mathbf{X}=\mathbf{I}$ and $\mathbf{\Theta}=\mathbf{V}_\mathrm{B}\mathbf{U}_\mathrm{F}^\mathsf{H}$. On the other hand, the lower bound is attained when the singular values of $\tilde{\mathbf{F}}$ and $\tilde{\mathbf{B}}$ are matched in reverse order, namely $\mathbf{X}=\mathbf{J}$ and $\mathbf{\Theta}=\mathbf{V}_\mathrm{B}\mathbf{J}\mathbf{U}_\mathrm{F}^\mathsf{H}$.

[21] One may think to take the *maximum* of those upper bounds as the problem of interest is the attainable dynamic range of n-th singular value. However, this is infeasible since the singular values will be reordered therein.

G. Proof of Corollary 3.6

When perfect CSI is available at the transmitter, in the low-SNR regime, the capacity is achieved by dominant eigenmode transmission [54, (5.26)]

$$\begin{aligned}C_{\rho_\downarrow} &= \log\left(1+\rho\lambda_1(\mathbf{H}^\mathsf{H}\mathbf{H})\right) \\ &= \log\left(1+\rho\sigma_1^2(\mathbf{H})\right) \\ &\approx \rho\sigma_1^2(\mathbf{H}) \\ &\leq \rho\sigma_1^2(\mathbf{H}_\mathrm{B})\sigma_1^2(\mathbf{H}_\mathrm{F}),\end{aligned}$$

where the approximation is $\log(1+x)\approx x$ for small x and the inequality follows from (13a) with $k=1$. In the high-SNR regime, the capacity is achieved by multiple eigenmode transmission with uniform power location [54, (5.27)]

$$\begin{aligned}C_{\rho_\uparrow} &= \sum\nolimits_{n=1}^{N}\log\left(1+\frac{\rho}{N}\lambda_n(\mathbf{H}^\mathsf{H}\mathbf{H})\right) \\ &\approx \sum\nolimits_{n=1}^{N}\log\left(\frac{\rho}{N}\sigma_n^2(\mathbf{H})\right) \\ &= N\log\frac{\rho}{N} + \sum\nolimits_{n=1}^{N}\log\sigma_n^2(\mathbf{H}) \\ &= N\log\frac{\rho}{N} + \log\prod\nolimits_{n=1}^{N}\sigma_n^2(\mathbf{H}) \\ &\leq N\log\frac{\rho}{N} + 2\log\prod\nolimits_{n=1}^{N}\sigma_n(\mathbf{H}_\mathrm{B})\sigma_n(\mathbf{H}_\mathrm{F}),\end{aligned}$$

where the approximation is $\log(1+x)\approx\log(x)$ for large x and the inequality follows from (13a) with $k=N$.

We now show (23) can achieve the upper bounds in (24a) and (24b) simultaneously. On the one hand, (23) is a special case of (15a) with $\mathbf{P}=\mathbf{I}$, which satisfies (16a) and (17a) for $n=1$ and thus attain $\sigma_1(\mathbf{H})=\sigma_1(\mathbf{H}_\mathrm{B})\sigma_1(\mathbf{H}_\mathrm{F})$. On the other hand, since $\log(\cdot)$ is a monotonic function, we can prove similar to Appendix F that $\sum_{n=1}^{N}\log\sigma_n^2(\mathbf{H}) \leq \sum_{n=1}^{N}\log\sigma_n^2(\mathbf{H}_\mathrm{B})\sigma_n^2(\mathbf{H}_\mathrm{F})$ and the bound is tight at (23). The proof is complete.

H. Proof of Proposition 4

The sub-differential of a symmetric gauge function of singular values of a matrix with respect to the matrix itself is given by [55, Theorem 2]

$$\partial_{\mathbf{H}^*} f\left(\mathrm{sv}(\mathbf{H})\right) = \mathrm{conv}\left\{\mathbf{U}\mathbf{D}\mathbf{V}^\mathsf{H}\right\}, \quad (69)$$

where $\mathbf{D}\in\mathbb{C}^{N_\mathrm{R}\times N_\mathrm{T}}$ is a rectangular diagonal matrix with $[\mathbf{D}]_{n,n} \in \partial_{\sigma_n(\mathbf{H})} f\left(\mathrm{sv}(\mathbf{H})\right)$, $\forall n\in[N]$, and $\mathbf{U}$, $\mathbf{V}$ are any left and right singular matrices of $\mathbf{H}$. It implies

$$\begin{aligned}\partial f\left(\mathrm{sv}(\mathbf{H})\right) &\ni \mathrm{tr}\left(\mathbf{V}^*\mathbf{D}^\mathsf{T}\mathbf{U}^\mathsf{T}\partial\mathbf{H}^*\right) \\ &= \mathrm{tr}\left(\mathbf{V}^*\mathbf{D}^\mathsf{T}\mathbf{U}^\mathsf{T}\mathbf{H}_{\mathrm{B},g}^*\partial\mathbf{\Theta}_g^*\mathbf{H}_{\mathrm{F},g}^*\right) \\ &= \mathrm{tr}\left(\mathbf{H}_{\mathrm{F},g}^*\mathbf{V}^*\mathbf{D}^\mathsf{T}\mathbf{U}^\mathsf{T}\mathbf{H}_{\mathrm{B},g}^*\partial\mathbf{\Theta}_g^*\right),\end{aligned}$$

and therefore $\mathbf{H}_{\mathrm{B},g}^\mathsf{H}\mathbf{U}\mathbf{D}\mathbf{V}^\mathsf{H}\mathbf{H}_{\mathrm{F},g}^\mathsf{H}$ constitutes a sub-gradient of $f\left(\mathrm{sv}(\mathbf{H})\right)$ with respect to $\mathbf{\Theta}_g$. The convex hull of those sub-gradients is the sub-differential (26).

I. Proof of Lemma 1

The differential of R with respect to $\mathbf{\Theta}_g^*$ is [70]

$$\begin{aligned}\partial R &= \frac{1}{\eta}\mathrm{tr}\Big\{\partial\mathbf{H}^* \cdot \mathbf{Q}^\mathsf{T}\mathbf{H}^\mathsf{T}\Big(\mathbf{I}+\frac{\mathbf{H}^*\mathbf{Q}^\mathsf{T}\mathbf{H}^\mathsf{T}}{\eta}\Big)^{-1}\Big\} \\ &= \frac{1}{\eta}\mathrm{tr}\Big\{\mathbf{H}_{\mathrm{B},g}^* \cdot \partial\mathbf{\Theta}_g^* \cdot \mathbf{H}_{\mathrm{F},g}^*\mathbf{Q}^\mathsf{T}\mathbf{H}^\mathsf{T}\Big(\mathbf{I}+\frac{\mathbf{H}^*\mathbf{Q}^\mathsf{T}\mathbf{H}^\mathsf{T}}{\eta}\Big)^{-1}\Big\} \\ &= \frac{1}{\eta}\mathrm{tr}\Big\{\mathbf{H}_{\mathrm{F},g}^*\mathbf{Q}^\mathsf{T}\mathbf{H}^\mathsf{T}\Big(\mathbf{I}+\frac{\mathbf{H}^*\mathbf{Q}^\mathsf{T}\mathbf{H}^\mathsf{T}}{\eta}\Big)^{-1}\mathbf{H}_{\mathrm{B},g}^* \cdot \partial\mathbf{\Theta}_g^*\Big\},\end{aligned}$$

and the corresponding complex derivative is (37).

J. Proof of Proposition 5

The differential of (39a) with respect to $\mathbf{\Theta}_g^*$ is

$$\begin{aligned}\partial\|\mathbf{H}\|_\mathrm{F}^2 &= \mathrm{tr}\big(\mathbf{H}_{\mathrm{B},g}^* \cdot \partial\mathbf{\Theta}_g^* \cdot \mathbf{H}_{\mathrm{F},g}^*(\mathbf{H}_\mathrm{D}^\mathsf{T}+\mathbf{H}_\mathrm{F}^\mathsf{T}\mathbf{\Theta}^\mathsf{T}\mathbf{H}_\mathrm{B}^\mathsf{T})\big) \\ &= \mathrm{tr}\big(\mathbf{H}_{\mathrm{F},g}^*(\mathbf{H}_\mathrm{D}^\mathsf{T}+\mathbf{H}_\mathrm{F}^\mathsf{T}\mathbf{\Theta}^\mathsf{T}\mathbf{H}_\mathrm{B}^\mathsf{T})\mathbf{H}_{\mathrm{B},g}^* \cdot \partial\mathbf{\Theta}_g^*\big)\end{aligned}$$

and the corresponding complex derivative is

$$\frac{\partial\|\mathbf{H}\|_\mathrm{F}^2}{\partial\mathbf{\Theta}_g^*} = \mathbf{H}_{\mathrm{B},g}^\mathsf{H}(\mathbf{H}_\mathrm{D}+\mathbf{H}_\mathrm{B}\mathbf{\Theta}\mathbf{H}_\mathrm{F})\mathbf{H}_{\mathrm{F},g}^\mathsf{H} \triangleq \mathbf{M}_g, \tag{70}$$

whose SVD is denoted as $\mathbf{M}_g = \mathbf{U}_g\mathbf{\Sigma}_g\mathbf{V}_g^\mathsf{H}$. The quadratic objective (39a) can be successively approximated by its first-order Taylor expansion, resulting in the subproblem

$$\max_{\mathbf{\Theta}} \quad \sum_g 2\Re\big\{\mathrm{tr}(\mathbf{\Theta}_g^\mathsf{H}\mathbf{M}_g)\big\} \tag{71a}$$

$$\text{s.t.} \quad \mathbf{\Theta}_g^\mathsf{H}\mathbf{\Theta}_g = \mathbf{I}, \quad \forall g, \tag{71b}$$

whose optimal solution is

$$\tilde{\mathbf{\Theta}}_g = \mathbf{U}_g\mathbf{V}_g^\mathsf{H}, \quad \forall g. \tag{72}$$

This is because $\Re\big\{\mathrm{tr}(\mathbf{\Theta}_g^\mathsf{H}\mathbf{M}_g)\big\} = \Re\big\{\mathrm{tr}(\mathbf{\Sigma}_g\mathbf{V}_g^\mathsf{H}\mathbf{\Theta}_g^\mathsf{H}\mathbf{U}_g)\big\} \leq \mathrm{tr}(\mathbf{\Sigma}_g)$ and the bound is tight when $\mathbf{V}_g^\mathsf{H}\mathbf{\Theta}_g^\mathsf{H}\mathbf{U}_g = \mathbf{I}$.

Next, we prove that solving the affine approximation (71) by (72) does not decrease (39a). Since $\tilde{\mathbf{\Theta}} = \mathrm{diag}(\tilde{\mathbf{\Theta}}_1,...,\tilde{\mathbf{\Theta}}_G)$ is optimal for (71), we have

$$\begin{aligned}&2\Re\Big\{\sum_g \mathrm{tr}(\tilde{\mathbf{\Theta}}_g^\mathsf{H}\mathbf{H}_{\mathrm{B},g}^\mathsf{H}\mathbf{H}_\mathrm{D}\mathbf{H}_{\mathrm{F},g}^\mathsf{H}) \\ &\qquad + \sum_{g_1,g_2}\mathrm{tr}(\tilde{\mathbf{\Theta}}_{g_1}^\mathsf{H}\mathbf{H}_{\mathrm{B},g_1}^\mathsf{H}\mathbf{H}_{\mathrm{B},g_2}\mathbf{\Theta}_{g_2}\mathbf{H}_{\mathrm{F},g_2}\mathbf{H}_{\mathrm{F},g_1}^\mathsf{H})\Big\} \\ &\geq 2\Re\Big\{\sum_g \mathrm{tr}(\mathbf{\Theta}_g^\mathsf{H}\mathbf{H}_{\mathrm{B},g}^\mathsf{H}\mathbf{H}_\mathrm{D}\mathbf{H}_{\mathrm{F},g}^\mathsf{H}) \\ &\qquad + \sum_{g_1,g_2}\mathrm{tr}(\mathbf{\Theta}_{g_1}^\mathsf{H}\mathbf{H}_{\mathrm{B},g_1}^\mathsf{H}\mathbf{H}_{\mathrm{B},g_2}\mathbf{\Theta}_{g_2}\mathbf{H}_{\mathrm{F},g_2}\mathbf{H}_{\mathrm{F},g_1}^\mathsf{H})\Big\}.\end{aligned} \tag{73}$$

Besides, $\|\sum_g\mathbf{H}_{\mathrm{B},g}\tilde{\mathbf{\Theta}}_g\mathbf{H}_{\mathrm{F},g} - \sum_g\mathbf{H}_{\mathrm{B},g}\mathbf{\Theta}_g\mathbf{H}_{\mathrm{F},g}\|_\mathrm{F}^2 \geq 0$ implies

$$\begin{aligned}&\sum_{g_1,g_2}\mathrm{tr}(\mathbf{H}_{\mathrm{F},g_1}^\mathsf{H}\tilde{\mathbf{\Theta}}_{g_1}^\mathsf{H}\mathbf{H}_{\mathrm{B},g_1}^\mathsf{H}\mathbf{H}_{\mathrm{B},g_2}\tilde{\mathbf{\Theta}}_{g_2}\mathbf{H}_{\mathrm{F},g_2}) \\ &\qquad + \sum_{g_1,g_2}\mathrm{tr}(\mathbf{H}_{\mathrm{F},g_1}^\mathsf{H}\mathbf{\Theta}_{g_1}^\mathsf{H}\mathbf{H}_{\mathrm{B},g_1}^\mathsf{H}\mathbf{H}_{\mathrm{B},g_2}\mathbf{\Theta}_{g_2}\mathbf{H}_{\mathrm{F},g_2}) \\ &\geq 2\Re\Big\{\sum_{g_1,g_2}\mathrm{tr}(\mathbf{H}_{\mathrm{F},g_1}^\mathsf{H}\tilde{\mathbf{\Theta}}_{g_1}^\mathsf{H}\mathbf{H}_{\mathrm{B},g_1}^\mathsf{H}\mathbf{H}_{\mathrm{B},g_2}\mathbf{\Theta}_{g_2}\mathbf{H}_{\mathrm{F},g_2})\Big\}.\end{aligned} \tag{74}$$

Adding (73) and (74), we have

$$\begin{aligned}&2\Re\big\{\mathrm{tr}(\tilde{\mathbf{\Theta}}^\mathsf{H}\mathbf{H}_\mathrm{B}^\mathsf{H}\mathbf{H}_\mathrm{D}\mathbf{H}_\mathrm{F}^\mathsf{H})\big\} + \mathrm{tr}(\mathbf{H}_\mathrm{F}^\mathsf{H}\tilde{\mathbf{\Theta}}^\mathsf{H}\mathbf{H}_\mathrm{B}^\mathsf{H}\mathbf{H}_\mathrm{B}\tilde{\mathbf{\Theta}}\mathbf{H}_\mathrm{F}) \\ &\geq 2\Re\big\{\mathrm{tr}(\mathbf{\Theta}^\mathsf{H}\mathbf{H}_\mathrm{B}^\mathsf{H}\mathbf{H}_\mathrm{D}\mathbf{H}_\mathrm{F}^\mathsf{H})\big\} + \mathrm{tr}(\mathbf{H}_\mathrm{F}^\mathsf{H}\mathbf{\Theta}^\mathsf{H}\mathbf{H}_\mathrm{B}^\mathsf{H}\mathbf{H}_\mathrm{B}\mathbf{\Theta}\mathbf{H}_\mathrm{F}),\end{aligned} \tag{75}$$

which suggests that (39a) is non-decreasing as the solution iterates over (72). Since (39a) is also bounded from above, the sequence of objective values converges.

Finally, we prove that any solution when (39a) converges, denoted by $\tilde{\mathbf{\Theta}}^?$, is a stationary point of (39). The Karush-Kuhn-Tucker (KKT) conditions of (39) and (71) are equivalent in terms of primal/dual feasibility and complementary slackness, while the stationary conditions are respectively, $\forall g$,

$$\mathbf{H}_{\mathrm{B},g}^\mathsf{H}(\mathbf{H}_\mathrm{D}+\mathbf{H}_\mathrm{B}\mathbf{\Theta}^\star\mathbf{H}_\mathrm{F})\mathbf{H}_{\mathrm{F},g}^\mathsf{H} - \mathbf{\Theta}_g^\star\mathbf{\Lambda}_g^\mathsf{H} = 0, \tag{76}$$

$$\mathbf{M}_g - \mathbf{\Theta}_g^\star\mathbf{\Lambda}_g^\mathsf{H} = 0. \tag{77}$$

On convergence of (39a), we have $\|\mathbf{H}_\mathrm{D}+\mathbf{H}_\mathrm{B}\mathbf{\Theta}^?\mathbf{H}_\mathrm{F}\|_\mathrm{F}^2$

(77) becomes $\mathbf{H}_{\mathrm{B},g}^\mathsf{H}(\mathbf{H}_\mathrm{D} + \mathbf{H}_\mathrm{B}\mathbf{\Theta}^?\mathbf{H}_\mathrm{F})\mathbf{H}_{\mathrm{F},g}^\mathsf{H} - \mathbf{\Theta}_g^?\mathbf{\Lambda}_g^\mathsf{H} = 0$ and reduces to (76). The proof is thus completed.

K. Proof of Lemma 2

The differential of $f = \sum_{k=1}^K \rho_k R_k$ with respect to $\mathbf{\Theta}_g^*$ is

$$\begin{aligned}\partial f = &\sum_{k=1}^K \rho_k \mathrm{tr}\Big\{\mathbf{E}_k\mathbf{W}_k^\mathsf{H}\Big(\mathbf{H}_{\mathrm{F},g}^{(k)\mathsf{H}}\partial\mathbf{\Theta}_g^\mathsf{H}\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\mathbf{Q}_k^{(-1)}\mathbf{H}^{(kk)} \\ &+\mathbf{H}^{(kk)\mathsf{H}}\mathbf{Q}_k^{(-1)}\mathbf{H}_{\mathrm{B},g}^{(k)}\partial\mathbf{\Theta}_g\mathbf{H}_{\mathrm{F},g}^{(k)} - \mathbf{H}^{(kk)\mathsf{H}}\mathbf{Q}_k^{(-1)} \\ &\times\sum_{j\neq k}\Big(\mathbf{H}_{\mathrm{B},g}^{(k)}\partial\mathbf{\Theta}_g\mathbf{H}_{\mathrm{F},g}^{(j)}\mathbf{W}_j\mathbf{W}_j^\mathsf{H}\mathbf{H}^{(kj)\mathsf{H}} \\ &+\mathbf{H}^{(kj)}\mathbf{W}_j\mathbf{W}_j^\mathsf{H}\mathbf{H}_{\mathrm{F},g}^{(j)\mathsf{H}}\partial\mathbf{\Theta}_g^\mathsf{H}\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\Big)\mathbf{Q}_k^{(-1)}\mathbf{H}^{(kk)}\Big)\mathbf{W}_k\Big\} \\ = &\sum_{k=1}^K \rho_k\Big(\mathrm{tr}\Big\{\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\mathbf{Q}_k^{(-1)}\mathbf{H}^{(kk)}\mathbf{W}_k\mathbf{E}_k\mathbf{W}_k^\mathsf{H}\mathbf{H}_{\mathrm{F},g}^{(k)\mathsf{H}}\partial\mathbf{\Theta}_g^\mathsf{H}\Big\} \\ &+\mathrm{tr}\Big\{\mathbf{H}_{\mathrm{F},g}^{(k)\mathsf{H}}\mathbf{W}_k\mathbf{E}_k\mathbf{W}_k^\mathsf{H}\mathbf{H}^{(kk)\mathsf{H}}\mathbf{Q}_k^{(-1)}\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\partial\mathbf{\Theta}_g\Big\} \\ &-\mathrm{tr}\Big\{\sum_{j\neq k}\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\mathbf{Q}_k^{(-1)}\mathbf{H}^{(kk)}\mathbf{W}_k\mathbf{E}_k\mathbf{W}_k^\mathsf{H}\mathbf{H}^{(kk)\mathsf{H}} \\ &\quad\times\mathbf{Q}_k^{(-1)}\mathbf{H}^{(kj)}\mathbf{W}_j\mathbf{W}_j^\mathsf{H}\mathbf{H}_{\mathrm{F},g}^{(j)\mathsf{H}}\partial\mathbf{\Theta}_g^\mathsf{H}\Big\} \\ &-\mathrm{tr}\Big\{\sum_{j\neq k}\mathbf{H}_{\mathrm{F},g}^{(j)\mathsf{H}}\mathbf{W}_j\mathbf{W}_j^\mathsf{H}\mathbf{H}^{(kj)\mathsf{H}}\mathbf{Q}_k^{(-1)}\mathbf{H}^{(kk)}\mathbf{W}_k \\ &\quad\times\mathbf{E}_k\mathbf{W}_k^\mathsf{H}\mathbf{H}^{(kk)\mathsf{H}}\mathbf{Q}_k^{(-1)}\mathbf{H}_{\mathrm{B},g}^{(k)}\partial\mathbf{\Theta}_g\Big\}\Big),\end{aligned}$$

and the corresponding complex derivative is (48).

L. Proof of Proposition 6

Minimizing (53a) is equivalent to maximizing

$$
\begin{aligned}
f(\boldsymbol{\Theta}) =& -I+\sum_{g}\beta_{g}^{(k)}\mathrm{tr}\left\{\mathbf{H}_{\mathrm{F},g}^{(j)\mathsf{H}}\mathbf{H}_{\mathrm{F},g}^{(j)}\right\}\\
=& \sum_{k=1}^{K}\sum_{j\neq k}-\mathrm{tr}\left\{\sum_{g}\mathbf{H}_{\mathrm{F},g}^{(j)}\mathbf{H}_{\mathrm{D}}^{(kj)\mathsf{H}}\mathbf{H}_{\mathrm{B},g}^{(k)}\boldsymbol{\Theta}_{g}\right\}\\
&-\mathrm{tr}\left\{\sum_{g}\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\mathbf{H}_{\mathrm{D}}^{(kj)}\mathbf{H}_{\mathrm{F},g}^{(j)\mathsf{H}}\boldsymbol{\Theta}_{g}^{\mathsf{H}}\right\}\\
&-\mathrm{tr}\left\{\sum_{g_1=1}^{G}\sum_{g_2\neq g_1}\mathbf{H}_{\mathrm{B},g_2}^{(k)\mathsf{H}}\mathbf{H}_{\mathrm{B},g_1}^{(k)}\boldsymbol{\Theta}_{g_1}\mathbf{H}_{\mathrm{F},g_1}^{(j)}\mathbf{H}_{\mathrm{F},g_2}^{(j)\mathsf{H}}\boldsymbol{\Theta}_{g_2}^{\mathsf{H}}\right\}\\
&-\mathrm{tr}\left\{\sum_{g}\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\mathbf{H}_{\mathrm{B},g}^{(k)}\boldsymbol{\Theta}_{g}\mathbf{H}_{\mathrm{F},g}^{(j)\mathsf{H}}\mathbf{H}_{\mathrm{F},g}^{(j)}\boldsymbol{\Theta}_{g}^{\mathsf{H}}\right\}\\
&+\mathrm{tr}\left\{\sum_{g}\beta_{g}^{(k)}\boldsymbol{\Theta}_{g}\mathbf{H}_{\mathrm{F},g}^{(j)\mathsf{H}}\mathbf{H}_{\mathrm{F},g}^{(j)}\boldsymbol{\Theta}_{g}^{\mathsf{H}}\right\}\\
=& \sum_{k=1}^{K}\sum_{j\neq k}-\mathrm{tr}\left\{\sum_{g}\mathbf{H}_{\mathrm{F},g}^{(j)}\mathbf{H}_{\mathrm{D}}^{(kj)\mathsf{H}}\mathbf{H}_{\mathrm{B},g}^{(k)}\boldsymbol{\Theta}_{g}\right\}\\
&-\mathrm{tr}\left\{\sum_{g}\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\mathbf{H}_{\mathrm{D}}^{(kj)}\mathbf{H}_{\mathrm{F},g}^{(j)\mathsf{H}}\boldsymbol{\Theta}_{g}^{\mathsf{H}}\right\}\\
&-\mathrm{tr}\left\{\sum_{g_1=1}^{G}\sum_{g_2\neq g_1}\mathbf{H}_{\mathrm{B},g_2}^{(k)\mathsf{H}}\mathbf{H}_{\mathrm{B},g_1}^{(k)}\boldsymbol{\Theta}_{g_1}\mathbf{H}_{\mathrm{F},g_1}^{(j)}\mathbf{H}_{\mathrm{F},g_2}^{(j)\mathsf{H}}\boldsymbol{\Theta}_{g_2}^{\mathsf{H}}\right\}\\
&+\mathrm{tr}\left\{\sum_{g}\mathbf{B}_{g}^{(k)}\boldsymbol{\Theta}_{g}\mathbf{H}_{\mathrm{F},g}^{(j)\mathsf{H}}\mathbf{H}_{\mathrm{F},g}^{(j)}\boldsymbol{\Theta}_{g}^{\mathsf{H}}\right\},
\end{aligned}
$$

where $\mathbf{B}_{g}^{(k)}=\beta_{g}^{(k)}\mathbf{I}-\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\mathbf{H}_{\mathrm{B},g}^{(k)}$ and the relaxation constant $\beta_{g}^{(k)}$ can be chosen arbitrarily. One can choose $\beta_{g}^{(k)}=\lambda_1(\mathbf{H}_{\mathrm{B},g}^{(k)\mathsf{H}}\mathbf{H}_{\mathrm{B},g}^{(k)})$ to ensure the positive semi-definiteness of $\mathbf{B}_{g}^{(k)}$ and formulate a quadratic function to be maximized. The remaining proof is similar to Appendix J and omitted here.

Acknowledgement

The authors would like to thank the anonymous reviewers for their insightful criticisms and suggestions that helped us correct some technical errors and improve the clarity of the manuscript.

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