Channel Shaping Using Reconfigurable Intelligent Surfaces: From Diagonal to Beyond

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Abstract—This paper investigates how a passive Reconfigurable Intelligent Surface (RIS) can reshape the Multiple-Input Multiple-Output (MIMO) point-to-point channel in terms of singular values. We depart from the widely-adapted diagonal phase shift model to a general Beyond-Diagonal (BD) architecture, which provides superior shaping capability thanks to in-group connections between elements. An efficient Riemannian Conjugate Gradient (RCG) algorithm is tailored for smooth optimization problems of asymmetric BD-RIS with arbitrary group size, then invoked for the Pareto frontier of channel singular values. To understand the gain from off-diagonal entries, we also derive analytical singular value bounds in Line-of-Sight (LoS) and fully-connected scenarios. As a side product, we tackle MIMO rate maximization problem by alternating between active beamformer (eigenmode transmission) and passive beamformer (RCG algorithm) until convergence. A low-complexity suboptimal solution based on channel shaping is also proposed, where the decoupled problem is formulated as channel power maximization and solved in closed form iteratively. Theoretical analysis and numerical evaluation reveal that the shaping advantage of BD-RIS increases with group size and MIMO dimensions, stemming from stronger subchannel rearrangement and subspace alignment capabilities.

Index Terms—Reconfigurable intelligent surface, multi-input multi-output, manifold optimization, singular value control, rate maximization.

I. Introduction

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 serves on demand. This is empowered by the recent advances in Reconfigurable Intelligent Surface (RIS), a real-time programmable metasurface of numerous non-resonant sub-wavelength scattering elements. It can manipulate the amplitude, phase, frequency, and polarization of the scattered waves [1] with a higher energy efficiency, lower cost, lighter footprint, and greater scalability than relays. Using RIS for passive beamforming has attracted significant interest in wireless communication [2]-[5], backscatter [6], [7], sensing [8], [9], and power transfer literature [10]–[12], reporting a second-order array gain and fourth-order power scaling law (with proper waveform). On the other hand, RIS also enables backscatter modulation by dynamically switching between different patterns, as already investigated [13]-[15] and prototyped [16], [17]. Despite fruitful outcomes, one critical unanswered question is the channel shaping capability: To what extent can a passive RIS reshape the wireless channel?

The answer indeed depends on the hardware architecture and scattering model. In conventional (a.k.a. diagonal) RIS, each scattering element is tuned by a dedicated impedance and acts as an *individual* phase shifter [18]. The concept is generalized

to Beyond-Diagonal (BD)-RIS [19], [20] which groups adjacent elements using passive components. This allows *cooperative* scattering — wave impinging on one element can propagate within the circuit and depart partially from any element in the same group. BD-RIS can thus control both amplitude and phase of the reflected wave, generalizing the scattering matrix from diagonal with unit-magnitude entries to block diagonal with unitary blocks. Its benefit has been recently shown in receive power maximization [21]–[24], transmit power minimization [25], and rate maximization [24]–[28]. Practical issues such as channel estimation [29] and mutual coupling [30] have also been investigated. Therefore, BD-RIS is envisioned as the next generation channel shaper with stronger signal processing flexibility [31].

Channel shaping is different from passive beamforming as it seeks to modify the inherent properties of the channel itself. This allows one to decouple the RIS-transceiver design and explore the fundamental limits of channel manipulation. For example, diagonal RIS has been proved useful for improving channel power [32], degree of freedom [33], [34], condition number [35], [36], and effective rank [37], [38] in Multiple-Input Multiple-Output (MIMO). In contrast, BD-RIS can provide a higher channel power but existing results are limited to Single-Input Single-Output (SISO)¹. [21] and Multiple-Input Single-Output (MISO) [22]. While these studies offer promising glimpses into the channel shaping potential, a comprehensive understanding of the capabilities and limitations is desired, and a universal design framework is missing. This paper aims to answer the channel shaping question through theoretical analysis and numerical optimization. The contributions are summarized below.

First, we quantify the capability of a BD-RIS to reshape the MIMO point-to-point channel in terms of singular values. The *Pareto frontiers* are characterized by optimizing the weighted sum of singular values, where the weights can be positive, zero, or negative. The resulting singular value region generalizes most relevant metrics and provides an intuitive channel shaping benchmark. We then discuss some analytical singular value bounds in Line-of-Sight (LoS) and fully-connected scenarios, which help to demystify the gain from off-diagonal entries. This is the first paper to answer the channel shaping question and highlight the BD-RIS gain from a Pareto perspective.

Second, we propose a Riemannian Conjugate Gradient (RCG) algorithm adapted from [39], [40] for smooth optimization problems of asymmetric BD-RIS with arbitrary

¹In terms of channel shaping, single-stream MIMO with given precoder and combiner [21] is equivalent to SISO.

group size. Specifically, block-wise update is performed along the geodesics² of the Stiefel manifold, which are expressed compactly by the exponential map [41]. It features lower complexity and faster convergence than general manifold optimization [42], [43], and solves the Pareto singular value problem. This is the first paper to tailor an efficient optimization framework for asymmetric BD-RIS.

Third, we tackle BD-RIS MIMO rate maximization with two solutions: a local-optimal approach through Alternating Optimization (AO) and a low-complexity approach over channel shaping. The former updates active and passive beamformers by eigenmode transmission and RCG algorithm, respectively. The latter suboptimally decouples both blocks, recasts the shaping problem as channel power maximization, and solves it iteratively in closed form. Interestingly, the gap in between vanishes as BD-RIS evolves from diagonal (single-connected) to unitary (fully-connected). It suggests channel shaping offers a promising low-complexity solution for joint RIS-transceiver designs.

Fourth, extensive simulations reveal that the performance gain from BD-RIS increases with group size and MIMO dimensions. In terms of channel power, fully-connected BD-RIS boosts up to 62%, 312%, 537% over single-connected in 1×1 , 4×4 , 16×16 MIMO under independent Rayleigh fading, respectively. The superiority stems from stronger subchannel rearrangement and subspace alignment capabilities empowered by in-group cooperation. It emphasizes the importance of using BD-RIS in large-scale MIMO systems.

Notation: Italic, bold lower-case, and bold upper-case letters indicate scalars, vectors and matrices, respectively. 3 denotes the imaginary unit. \mathbb{C} represents the set of complex numbers. $\mathbb{H}^{n\times n}$ and $\mathbb{U}^{n\times n}$ denotes the set of $n\times n$ Hermitian and unitary matrices, respectively. 0 and I are the all-zero and identity matrices with appropriate size, respectively. $\Re\{\cdot\}$ takes the real part of a complex number. $tr(\cdot)$ and $det(\cdot)$ evaluates the trace and determinant of a square matrix, respectively. $\operatorname{diag}(\cdot)$ constructs a square matrix with arguments on the main diagonal and zeros elsewhere. $sv(\cdot)$ returns the singular value vector. $\sigma_n(\cdot)$ and $\lambda_n(\cdot)$ is the *n*-th largest singular value and eigenvalue, respectively. $(\cdot)^*$, $(\cdot)^{\mathsf{T}}$, $(\cdot)^{\mathsf{H}}$, $(\cdot)^{\dagger}$ $(\cdot)^{(r)}$, $(\cdot)^*$ denote the conjugate, transpose, conjugate transpose (Hermitian), Moore-Penrose inverse, r-th iterated point, and final solution, respectively. $(\cdot)_{[x:y]}$ is a shortcut for $(\cdot)_x, (\cdot)_{x+1}, \dots, (\cdot)_y$. $|\cdot|$ denotes the absolute value. $\|\cdot\|$ means the Euclidean norm. $\|\cdot\|_{\mathrm{F}}$ represents the Frobenius norm. $\mathcal{CN}(\mathbf{0}, \Sigma)$ is the multivariate Circularly Symmetric Complex Gaussian (CSCG) distribution with mean 0 and covariance Σ . \sim means "distributed as".

II. BD-RIS MODEL

Consider a BD-RIS aided point-to-point MIMO system with $N_{\rm T}, N_{\rm S}, N_{\rm R}$ transmit, scatter, and receive antennas, respectively. This configuration is denoted as $N_{\rm T} \times N_{\rm S} \times N_{\rm R}$. The BD-RIS is modeled as an N_{S} -port network [44] that further divides into G individual groups. Each group contains $L \triangleq N_S/G$ elements interconnected by real-time reconfigurable components [19]. To simplify the analysis, we assume there are no mutual

coupling and the in-group connections can be lossless and asymmetric³. The overall scattering matrix is thus block diagonal $\Theta = \operatorname{diag}(\Theta_1, ..., \Theta_G) \in \mathbb{U}^{N_S \times N_S}$, where $\Theta_g \in \mathbb{U}^{L \times L}$ is a unitary matrix corresponding to group $g \in \mathcal{G} \triangleq \{1,...,G\}$. Let $\mathbf{H}_{\mathrm{D}} \in \mathbb{C}^{N_{\mathrm{R}} \times N_{\mathrm{T}}}$, $\mathbf{H}_{\mathrm{F}} \in \mathbb{C}^{N_{\mathrm{S}} \times N_{\mathrm{T}}}$, $\mathbf{H}_{\mathrm{B}} \in \mathbb{C}^{N_{\mathrm{R}} \times N_{\mathrm{S}}}$ denote the direct (transmitter-receiver), forward (transmitter-RIS), and backward (RIS-receiver) channels, respectively. The equivalent channel is

$$\mathbf{H} = \mathbf{H}_{\mathrm{D}} + \mathbf{H}_{\mathrm{B}} \mathbf{\Theta} \mathbf{H}_{\mathrm{F}} = \mathbf{H}_{\mathrm{D}} + \sum_{g} \mathbf{H}_{\mathrm{B},g} \mathbf{\Theta}_{g} \mathbf{H}_{\mathrm{F},g}, \qquad (1)$$

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 of RIS group q, respectively.

Remark 1. BD-RIS reduces to diagonal RIS and unitary RIS with group size 1 and $N_{\rm S}$, respectively.

Remark 2. Individual forward and backward Channel State Information (CSI) are required for BD-RIS designs. This is different from diagonal RIS where estimating their product is usually sufficient.

III. CHANNEL SINGULAR VALUES REDISTRIBUTION A. A Toy Example

We first illustrate the channel shaping capabilities of different RIS by a toy example. Consider a $2 \times 2 \times 2$ setup where the direct link is blocked. The diagonal RIS is modeled by $\Theta_{\rm D} = {\rm diag}(e^{j\theta_1}, e^{j\theta_2})$ while the unitary BD-RIS has 4 independent angular parameters

$$\Theta_{\rm U} = e^{\jmath\phi} \begin{bmatrix} e^{\jmath\alpha} \cos\psi & e^{\jmath\beta} \sin\psi \\ -e^{-\jmath\beta} \sin\psi & e^{-\jmath\alpha} \cos\psi \end{bmatrix}. \tag{2}$$

In particular, ϕ has no impact on the singular value because $\operatorname{sv}(e^{j\phi}\mathbf{A}) = \operatorname{sv}(\mathbf{A})$. We also enforce symmetry by $\beta = \pi/2$ such that both architectures have the same number of angular parameters. Fig. 1 shows the channel singular values achieved by an exhaustive grid search over (θ_1, θ_2) for diagonal RIS and (α, ψ) for symmetric unitary RIS. It is observed that both singular values can be manipulated up to 9\% using diagonal RIS and 42% using symmetric BD-RIS, despite both architectures have the same number of scattering elements and design parameters. A larger performance gap is expected when asymmetric BD-RIS is available. This example shows BD-RIS can provide a wider dynamic range of channel singular values and motivates further studies on channel shaping.

B. Pareto Frontier Characterization

We then characterize the Pareto frontier of channel singular values by maximizing their weighted sum

$$\max_{\mathbf{\Theta}} \quad \sum_{n} \rho_{n} \sigma_{n}(\mathbf{H})$$
 (3a)
s.t. $\mathbf{\Theta}_{g}^{\mathsf{H}} \mathbf{\Theta}_{g} = \mathbf{I}, \quad \forall g,$ (3b)

s.t.
$$\boldsymbol{\Theta}_{q}^{\mathsf{H}} \boldsymbol{\Theta}_{q} = \mathbf{I}, \quad \forall g,$$
 (3b)

where $n \in \{1,...,N \triangleq \min(N_T,N_R)\}$ and ρ_n is the weight of the n-th singular value that can be positive, zero, or negative.

³While symmetric impedance network is often considered in the literature [19], [21]-[27], asymmetric passive components (e.g., ring hybrids and branch-line hybrids) may also be reconfigured in real time [45]. Asymmetric BD-RIS has been discussed in [20], [27], [28].

²A geodesic refers to the shortest path between two points in a Riemannian manifold.

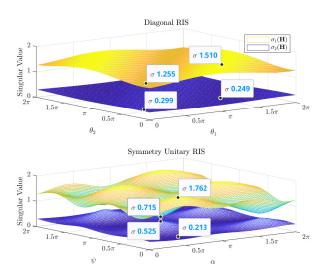


Fig. 1. $2 \times 2 \times 2$ (no direct) channel singular value shaping by diagonal and symmetry unitary RIS.

Varying $\{\rho_n\}$ unveils the entire achievable singular value region. Thus, the Pareto frontier problem (3) generalizes most relevant metrics and provides a powerful shaping framework. The objective (3a) is smooth in Θ and the feasible domain (3b) for group g corresponds to the Stiefel manifold. Next, we zoom out to general smooth maximization problems of asymmetric BD-RIS.

Inspired by [39], [40], we propose a block-wise RCG algorithm along the geodesics on the Lie group of unitary matrices $\mathbb{U}^{L\times L}$. It leverages the fact that unitary matrices are closed under multiplication. At iteration r, the gradient is computed in the Euclidean space and translated to the Riemannian manifold [42]

$$\nabla_{\mathrm{E},g}^{(r)} = \frac{\partial f(\mathbf{\Theta}_g^{(r)})}{\partial \mathbf{\Theta}_q^*},\tag{4}$$

$$\nabla_{{\rm R},g}^{(r)} \! = \! \nabla_{{\rm E},g}^{(r)} \! \boldsymbol{\Theta}_g^{(r)}{}^{\rm H} \! - \! \boldsymbol{\Theta}_g^{(r)} \! \nabla_{{\rm E},g}^{(r)} {}^{\rm H}. \eqno(5)$$

The Polak-Ribierre parameter [46] is approximated as [40]

$$\gamma_g^{(r)} = \frac{\text{tr}\left(\left(\nabla_{R,g}^{(r)} - \nabla_{R,g}^{(r-1)}\right)\nabla_{R,g}^{(r)}\right)}{\text{tr}\left(\nabla_{R,g}^{(r-1)}\nabla_{R,g}^{(r-1)}\right)},\tag{6}$$

and the conjugate direction is

$$\mathbf{D}_{g}^{(r)} = \nabla_{\mathbf{R},g}^{(r)} + \gamma_{g}^{(r)} \mathbf{D}_{g}^{(r-1)}.$$
 (7)

In the Stiefel manifold, the geodesic emanating from $\Theta_g^{(r)}$ with velocity $\mathbf{D}_g^{(r)}$ and step size μ is described compactly by the exponential map [41]

$$\mathbf{G}_{a}^{(r)}(\mu) = \exp(\mu \mathbf{D}_{a}^{(r)}) \mathbf{\Theta}_{a}^{(r)}. \tag{8}$$

An appropriate μ^* can be obtained by the Armijo rule [47].⁴ Finally, the scattering matrix is updated along the geodesic as

$$\mathbf{\Theta}_q^{(r+1)} = \mathbf{G}_q^{(r)}(\mu^*). \tag{9}$$

⁴To double the step size, one only need to square the rotation matrix instead of recomputing the matrix exponential, i.e., $\exp(2\mu\mathbf{D}_q^{(r)}) = \exp^2(\mu\mathbf{D}_q^{(r)})$.

Algorithm 1: Block-wise geodesic RCG for asymmetric BD-RIS

```
Input: f(\Theta), G
Output: O
   1: Initialize r \leftarrow 0, \boldsymbol{\Theta}^{(0)}
         Repeat
   2:
   3:
                   For g \leftarrow 1 to G
                            \nabla_{\mathrm{E},g}^{(r)} \leftarrow (4)
\nabla_{\mathrm{R},g}^{(r)} \leftarrow (5)
   4:
   5:
                             \gamma_q^{(r)} \leftarrow (6)
   6:
   7:
                           \begin{aligned} &\mathbf{If} \ \Re \big\{ \mathrm{tr}(\mathbf{D}_g^{(r)}^\mathsf{H} \nabla_{\mathrm{R},g}^{(r)}) \big\} < 0 \\ &\mathbf{D}_g^{(r)} \!\leftarrow\! \nabla_{\mathrm{R},g}^{(r)} \\ &\mathbf{End} \ \mathbf{If} \end{aligned}
   8:
                                                                                                            9:
 10:
11:
                             \mathbf{G}_{q}^{(r)}(\mu) \leftarrow (8)
12:
                             While f(\mathbf{G}_g^{(r)}(2\mu)) - f(\mathbf{\Theta}_g^{(r)}) \ge \mu \cdot \operatorname{tr}(\mathbf{D}_g^{(r)} \mathbf{D}_g^{(r)}^{\mathsf{H}})/2
13:
14:
                             End While
15:
                             While f(\mathbf{G}_q^{(r)}(\mu)) - f(\mathbf{\Theta}_q^{(r)}) < \mu/2 \cdot \text{tr}(\mathbf{D}_q^{(r)} \mathbf{D}_o^{(r)}^{\mathsf{H}})/2
16:
17:
                                     \mu \leftarrow \hat{\mu}/2
                            End While \Theta_g^{(r+1)} \leftarrow (9)
18:
19:
                   End For
20:
21:
22: Until |f(\boldsymbol{\Theta}^{(r)}) - f(\boldsymbol{\Theta}^{(r-1)})| / f(\boldsymbol{\Theta}^{(r-1)}) \le \epsilon
```

Algorithm 1 summarizes the proposed block-wise geodesic RCG method for smooth maximization problems of asymmetric BD-RIS. Convergence to stationary points is guaranteed.

Remark 3. Compared with universal manifold optimization [42], [43], Algorithm 1 inherits a trifold benefit from [39], [40]:

- 1) No retraction thanks to rotational update (8), (9);
- 2) Lower computational complexity per iteration;
- 3) Faster convergence thanks to proper parameter space.

Lemma 1. The Euclidean gradient of (3a) w.r.t. BD-RIS group g is

$$\frac{\partial \sum_{n} \rho_{n} \sigma_{n}(\mathbf{H})}{\partial \mathbf{\Theta}_{q}^{*}} = \mathbf{H}_{B,g}^{\mathsf{H}} \mathbf{U} \operatorname{diag}(\rho_{1}, ..., \rho_{N}) \mathbf{V}^{\mathsf{H}} \mathbf{H}_{F,g}^{\mathsf{H}}, \quad (10)$$

where U and V are the left and right singular matrices of H, respectively.

Proof. Please refer to Appendix A.
$$\Box$$

Algorithm 1 can thus be invoked for the Pareto singular value problem (3) where line 4 uses (10) explicitly.

C. Some Analytical Bounds

We then discuss some analytical bounds related to channel singular values.

Proposition 1 (degree of freedom). In point-to-point MIMO, BD-RIS cannot achieve a higher Degree of Freedom (DoF) than diagonal RIS.

Proposition 2 (rank-deficient channel). If the forward or backward channel is rank-k, then regardless of the RIS size

and architecture, the n-th singular value of the equivalent channel is bounded by

$$\sigma_n(\mathbf{H}) \le \sigma_{n-k}(\mathbf{T}), \quad if \ n > k,$$
 (11)

$$\sigma_n(\mathbf{H}) > \sigma_n(\mathbf{T}), \quad if \ n < N - k + 1, \quad (12)$$

where

$$\mathbf{T}\mathbf{T}^{\mathsf{H}} = \begin{cases} \mathbf{H}_{\mathsf{D}}(\mathbf{I} - \mathbf{V}_{\mathsf{F}}\mathbf{V}_{\mathsf{F}}^{\mathsf{H}})\mathbf{H}_{\mathsf{D}}^{\mathsf{H}}, & if \ \mathrm{rank}(\mathbf{H}_{\mathsf{F}}) = k, \\ \mathbf{H}_{\mathsf{D}}^{\mathsf{H}}(\mathbf{I} - \mathbf{U}_{\mathsf{B}}\mathbf{U}_{\mathsf{B}}^{\mathsf{H}})\mathbf{H}_{\mathsf{D}}, & if \ \mathrm{rank}(\mathbf{H}_{\mathsf{B}}) = k, \end{cases}$$
(13)

and $V_{\rm F}$ and $U_{\rm B}$ are the right and left compact singular matrices of \mathbf{H}_{F} and \mathbf{H}_{B} , respectively.

Corollary 2.1 (extreme singular values). With a sufficiently large RIS, the first k channel singular values are unbounded above while the last k channel singular values can be suppressed to zero.

Corollary 2.2 (LoS channel⁵). If the forward or backward channel is LoS, then a RIS can at most enlarge (resp. suppress) the n-th (n > 2) channel singular value to the (n-1)-th (resp. n-th) singular value of \mathbf{T} , that is,

$$\sigma_1(\mathbf{H}) \ge \sigma_1(\mathbf{T}) \ge \sigma_2(\mathbf{H}) \ge \dots \ge \sigma_{N-1}(\mathbf{T}) \ge \sigma_N(\mathbf{H}) \ge \sigma_N(\mathbf{T}). \tag{14}$$

In Section V, we will show by simulation that a finite-size BD-RIS can approach those bounds better than diagonal RIS.

Proposition 3 (fully-connected RIS without direct link). If the BD-RIS is fully-connected and the direct link is absent, then the channel singular values can be manipulated up to

$$sv(\mathbf{H}) = sv(\mathbf{BF}), \tag{15}$$

where B and F are arbitrary matrices with the same singular values as H_B and H_F, respectively,

The problem now becomes how the singular values of matrix product are bounded by the singular values of its individual factors. Let $N' = \max(N_T, N_S, N_R)$ and $\sigma_n(\mathbf{H}) = \sigma_n(\mathbf{H}_F) =$ $\sigma_n(\mathbf{H}_{\mathrm{B}}) = 0$ for $N < n \le N'$. We have the following corollaries.

Corollary 3.1 (generic singular value bounds [49]).

$$\prod_{k \in K} \sigma_k(\mathbf{H}) \le \prod_{i \in I} \sigma_i(\mathbf{H}_{\mathrm{B}}) \prod_{j \in J} \sigma_j(\mathbf{H}_{\mathrm{F}}), \tag{16}$$

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

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

$$\boldsymbol{U}_r^{N'} \triangleq \Bigl\{ (\boldsymbol{I}, \! \boldsymbol{J}, \! \boldsymbol{K}) \, | \, \sum_{i \in I} \! i + \! \sum_{j \in J} \! j = \sum_{k \in K} \! k + r(r+1)/2 \Bigr\}.$$

Corollary 3.2 (upper bound on the largest singular value).

$$\sigma_1(\mathbf{H}) \le \sigma_1(\mathbf{H}_{\mathrm{B}}) \sigma_1(\mathbf{H}_{\mathrm{F}}).$$
 (17)

Corollary 3.3 (upper bound on the product of first k singular

$$\prod_{n=1}^{k} \sigma_n(\mathbf{H}) \le \prod_{n=1}^{k} \sigma_n(\mathbf{H}_{\mathrm{B}}) \prod_{n=1}^{k} \sigma_n(\mathbf{H}_{\mathrm{F}}). \tag{18}$$

Corollary 3.4 (upper bound on the sum of first k singular values to the power of p).

$$\sum_{n=1}^{k} \sigma_n^p(\mathbf{H}) \le \sum_{n=1}^{k} \sigma_n^p(\mathbf{H}_{\mathrm{B}}) \sigma_n^p(\mathbf{H}_{\mathrm{F}}), \quad p > 0.$$
 (19)

When k = N' and p = 2, (19) suggests the channel power is upper bounded by the sum of (sorted) element-wise power product of backward and forward subchannels.

Remark 4. Interestingly, (16)–(19) are simultaneously tight when $\Theta = V_B U_F^H$. We thus conclude the off-diagonal entries can enhance the capabilities of

- subspace alignment: $V_{\rm B}$ and $U_{\rm F}^{\sf H}$ in (34) fully align the subspaces of \mathbf{H}_{B} and \mathbf{H}_{F} by rotation;
- subchannel rearrangement: X = I in (35) pairs the subchannels of H_B and H_F from strongest to weakest, which attains the maximal in rearrangement inequality.

Tight bounds are inapplicable when a MIMO direct link is present, as the RIS needs to balance the direct-indirect (additive) and backward-forward (multiplicative) subspace alignments. Such a balance often involves optimization approaches and another example will be discussed in Section IV-B.

IV. ACHIEVABLE RATE MAXIMIZATION

The MIMO achievable rate maximization problem is formulated w.r.t. joint active and passive beamforming

$$\max_{\mathbf{W},\Theta} R = \operatorname{logdet}\left(\mathbf{I} + \frac{\mathbf{W}^{\mathsf{H}}\mathbf{H}^{\mathsf{H}}\mathbf{H}\mathbf{W}}{\eta}\right) \qquad (20a)$$
s.t.
$$\|\mathbf{W}\|_{\mathrm{F}}^{2} \leq P, \qquad (20b)$$

s.t.
$$\|\mathbf{W}\|_{\mathrm{F}}^2 \le P$$
, (20b)

$$\Theta_a^{\mathsf{H}}\Theta_a = \mathbf{I}, \quad \forall g,$$
 (20c)

where W is the transmit precoder, R is the achievable rate, η is the noise power, and P is the transmit power budget. Two methods are proposed below to solve problem (20).

A. Alternating Optimization

Consider an AO approach that updates Θ and W iteratively. For a given W, the passive beamforming subproblem is

$$\max_{\mathbf{\Theta}} \quad \operatorname{logdet}\left(\mathbf{I} + \frac{\mathbf{H}\mathbf{Q}\mathbf{H}^{\mathsf{H}}}{\eta}\right) \tag{21a}$$

s.t.
$$\Theta_g^{\mathsf{H}}\Theta_g = \mathbf{I}, \quad \forall g,$$
 (21b)

where $\mathbf{Q} \triangleq \mathbf{W} \mathbf{W}^{\mathsf{H}}$ is the transmit covariance matrix.

Lemma 2. The Euclidean gradient of (21a) w.r.t. BD-RIS block g is

$$\frac{\partial R}{\partial \mathbf{\Theta}_{q}^{*}} = \frac{1}{\eta} \mathbf{H}_{\mathrm{B},g}^{\mathsf{H}} \left(\mathbf{I} + \frac{\mathbf{H} \mathbf{Q} \mathbf{H}^{\mathsf{H}}}{\eta} \right)^{-1} \mathbf{H} \mathbf{Q} \mathbf{H}_{\mathrm{F},g}^{\mathsf{H}}. \tag{22}$$

Proof. Please refer to Appendix E.

⁵A similar result has been derived for diagonal RIS in [48].

Algorithm 1 is then invoked to solve problem (20) where line 4 uses (22) explicitly. Since (21a) is a concave function of Θ , convergence to local-optimal points is guaranteed. On the other hand, the global optimal transmit precoder for a fixed Θ is given by the eigenmode transmission [50]

$$\mathbf{W}^{\star} = \mathbf{V} \mathbf{S}^{\star 1/2}, \tag{23}$$

where V is the right channel singular matrix and S^* is the optimal water-filling power allocation matrix. The overall AO algorithm converges to local-optimal points of problem (20) since each subproblem is solved optimally and the objective is bounded above.

B. Low-Complexity Solution

We then propose a low-complexity solution to problem (20) based on channel shaping. The passive beamforming subproblem (21) involves transmit covariance matrix Q and thus requires iterative RCG update. Instead, we decouple the joint RIS-transceiver design by recasting (21) as channel power maximization

$$\max_{\mathbf{\Theta}} \quad \|\mathbf{H}_{\mathrm{D}} + \mathbf{H}_{\mathrm{B}} \mathbf{\Theta} \mathbf{H}_{\mathrm{F}} \|_{\mathrm{F}}^{2}$$
s.t. $\mathbf{\Theta}_{g}^{\mathsf{H}} \mathbf{\Theta}_{g} = \mathbf{I}, \quad \forall g.$ (24a)

s.t.
$$\mathbf{\Theta}_q^{\mathsf{H}} \mathbf{\Theta}_g = \mathbf{I}, \quad \forall g.$$
 (24b)

Remark 5. As mentioned in Section III-C, the key of solving (24) is to balance the additive and multiplicative subspace alignments. Problem (24) is very similar (in terms of maximizing the inner product of H_D and $H_B\Theta H_F$) to the weighted orthogonal Procrustes problem [51]

$$\min_{\mathbf{\Theta}} \quad \|\mathbf{H}_{\mathrm{D}} - \mathbf{H}_{\mathrm{B}} \mathbf{\Theta} \mathbf{H}_{\mathrm{F}}\|_{\mathrm{F}}^{2} \tag{25a}$$
s.t. $\mathbf{\Theta}^{\mathsf{H}} \mathbf{\Theta} = \mathbf{I}$, (25b)

s.t.
$$\Theta^{\mathsf{H}}\Theta = \mathbf{I}$$
, (25b)

which has no trivial solution. One lossy transformation, by moving Θ to one side [52], formulates standard orthogonal Procrustes problems

$$\min_{\boldsymbol{\Theta}} \quad \|\boldsymbol{H}_{\mathrm{B}}^{\dagger}\boldsymbol{H}_{\mathrm{D}}\!-\!\boldsymbol{\Theta}\boldsymbol{H}_{\mathrm{F}}\|_{\mathrm{F}}^{2} \ \textit{or} \ \|\boldsymbol{H}_{\mathrm{D}}\boldsymbol{H}_{\mathrm{F}}^{\dagger}\!-\!\boldsymbol{H}_{\mathrm{B}}\boldsymbol{\Theta}\|_{\mathrm{F}}^{2} \quad \ \ \text{(26a)}$$

s.t.
$$\Theta^{\mathsf{H}}\Theta = \mathbf{I}$$
, (26b)

which has global optimal solutions $\Theta^* = UV^H$ where U and ${f V}$ are the left and right singular matrices of ${f H}_{
m B}^\dagger {f H}_{
m D} {f H}_{
m F}^{\sf H}$ or $\mathbf{H}_{\mathrm{B}}^{\mathsf{H}}\mathbf{H}_{\mathrm{D}}\mathbf{H}_{\mathrm{E}}^{\dagger}$ [53]. This naive solution will be compared with the one proposed below.

Inspired by [54], we successively approximate the quadratic objective (24a) by local Taylor expansions and solve each iteration in closed form.

Proposition 4. Start from any $\Theta^{(0)} \in \mathbb{U}^{N_S \times N_S}$, the sequence

$$\mathbf{\Theta}_{a}^{(r+1)} = \mathbf{U}_{a}^{(r)} \mathbf{V}_{a}^{(r)}, \quad \forall g$$
 (27)

converges to a stationary point of (24), where $\mathbf{U}_g^{(r)}$ and $\mathbf{V}_g^{(r)}$ are the left and right compact singular matrix of

$$\mathbf{M}_{g}^{(r)} = \mathbf{H}_{\mathrm{B},g}^{\mathsf{H}} \left(\mathbf{H}_{\mathrm{D}} + \mathbf{H}_{\mathrm{B}} \mathrm{diag} \left(\mathbf{\Theta}_{[1:g-1]}^{(r+1)}, \mathbf{\Theta}_{[g:G]}^{(r)} \right) \mathbf{H}_{\mathrm{F}} \right) \mathbf{H}_{\mathrm{F},g}^{\mathsf{H}}$$
(28)

Proof. Please refer to Appendix F.

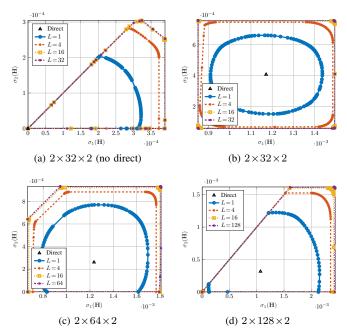


Fig. 2. Pareto frontiers of 2T2R channel singular values reshaped by a RIS.

Once the channel shaping problem (24) is solved, the transmit precoder can be obtained by (23). This two-stage approach decouples both blocks and is computationally efficient.

V. SIMULATION RESULTS

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

A. Channel Singular Values Redistribution

1) Pareto Frontier: Fig. 2 shows the Pareto singular values of a 2T2R MIMO reshaped by a RIS. When the direct link is absent, the achievable regions in Fig. 2(a) are shaped like pizza slices since $\sigma_1(\mathbf{H}) > \sigma_2(\mathbf{H}) > 0$. We observe that the smallest singular value is enhanced up to 2×10^{-4} by diagonal RIS and 3×10^{-4} by fully-connected BD-RIS, corresponding to a 50 % gain. When the direct link is present, the region shape depends heavily on the relative channel strength. In Fig. 2(b), a 32-element RIS cannot compensate the 35 dB direct-indirect power imbalance and results in a limited range of singular values. The achievable regions are thus symmetric around the direct point. Interestingly, the shape evolves from oval to square

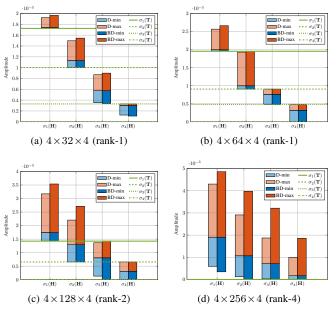


Fig. 3. Achievable channel singular values: analytical bounds (green lines) and numerical optimization results (blue and red bars). 'D' means diagonal RIS and 'BD' means fully-connected BD-RIS. 'rank-k' refers to the forward channel.

as the group size L increases, which suggests that BD-RIS can achieve a better tradeoff in subchannel manipulation. As the number of scattering elements $N_{\rm S}$ increases, the dynamic range of singular values is widened and the achievable region becomes more trapezoidal. It is also worth noticing in Fig. 2(d) that the equivalent channel can be completely nulled by a 128-element BD-RIS but not by a diagonal one. Those results demonstrate the superior channel shaping capability of BD-RIS and the importance of in-group connections.

2) Analytical and Numerical Results: Fig. 3 illustrates the analytical bounds in Proposition 2 and the numerical results obtained by solving problem (3) with $\rho_n = \pm 1$ and $\rho_{n'} = 0$, $\forall n' \neq n$. Here we assme 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 2.2, 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. We also observe that BD-RIS can approach those bounds better than diagonal RIS especially for a small $N_{\rm S}$. Another example is given in Fig. 3(c) where the forward channel is rank-2. As expected from Corollary 2.1, the largest 2 singular values are unbounded above and the smallest 2 singular values can be suppressed to zero (with a sufficiently large RIS). Proposition 2 also predicts the fact that $\sigma_1(\mathbf{H}) \geq \sigma_1(\mathbf{T}), \ \sigma_2(\mathbf{H}) \geq \sigma_2(\mathbf{T}), \ \sigma_3(\mathbf{H}) \leq \sigma_1(\mathbf{T}), \ \text{and}$ $\sigma_4(\mathbf{H}) \le \sigma_2(\mathbf{T})$. Finally, Fig. 3(d) confirms there are no extra bounds when both forward and backward channels are full-rank. This is because in (13) the compact singular matrices V_F and U_F become unitary such that T=0. The numerical results are consistent with the analytical bounds, and we also conclude that the advantage of BD-RIS over diagonal RIS scales with indirect channel ranks.

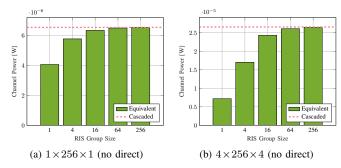


Fig. 4. Average channel power versus BD-RIS group size and MIMO dimensions.

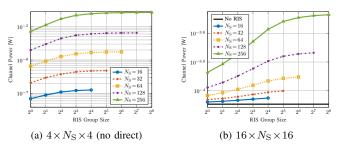


Fig. 5. Average channel power versus antenna size and BD-RIS group size.

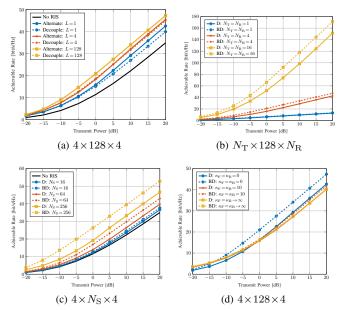


Fig. 6. Average channel power versus antenna size and BD-RIS group size.

B. Achievable Rate Maximization

APPENDIX

A. Proof of Lemma 1

Let $\mathbf{H} = \sum_n \mathbf{u}_n \sigma_n \mathbf{v}_n^{\mathsf{H}}$ be the compact Singular Value Decomposition (SVD) of the equivalent channel. Since the singular vectors are orthonormal, the *n*-th singular value can be expressed as

$$\sigma_n = \mathbf{u}_n^\mathsf{H} \mathbf{H} \mathbf{v}_n = \mathbf{u}_n^\mathsf{T} \mathbf{H}^* \mathbf{v}_n^*, \tag{29}$$

whose differential w.r.t. Θ_q^* is

$$\begin{split} \partial \sigma_n &= \partial \mathbf{u}_n^\mathsf{T} \underbrace{\mathbf{H}^* \mathbf{v}_n^*}_{\sum_m \mathbf{u}_m^* \sigma_m \mathbf{v}_m^\mathsf{T} \mathbf{v}_n} + \mathbf{u}_n^\mathsf{T} \cdot \partial \mathbf{H}^* \cdot \mathbf{v}_n^* + \underbrace{\mathbf{u}_n^\mathsf{T} \mathbf{H}^*}_{\mathbf{u}_n^\mathsf{T} \sum_m \mathbf{u}_m^* \sigma_m \mathbf{v}_n^\mathsf{T}}_{\partial \mathbf{v}_n^*} \partial \mathbf{v}_n^* \\ &= \underbrace{\partial \mathbf{u}_n^\mathsf{T} \mathbf{u}_n^* \cdot \sigma_n + \mathbf{u}_n^\mathsf{T} \cdot \partial \mathbf{H}^* \cdot \mathbf{v}_n^* + \sigma_n \cdot \underbrace{\mathbf{v}_n^\mathsf{T} \partial \mathbf{v}_n^*}_{\partial 1 = 0} \\ &= \mathbf{u}_n^\mathsf{T} \mathbf{H}_{B,g}^* \cdot \partial \mathbf{\Theta}_g^* \cdot \mathbf{H}_{F,g}^* \mathbf{v}_n^* \\ &= \operatorname{tr}(\mathbf{H}_{F,g}^* \mathbf{v}_n^* \mathbf{u}_n^\mathsf{T} \mathbf{H}_{B,g}^* \cdot \partial \mathbf{\Theta}_g^*). \end{split}$$

According to [55], the corresponding complex derivative is

$$\frac{\partial \sigma_n}{\partial \mathbf{\Theta}_q^*} = \mathbf{H}_{\mathrm{B},g}^{\mathsf{H}} \mathbf{u}_n \mathbf{v}_n^{\mathsf{H}} \mathbf{H}_{\mathrm{F},g}^{\mathsf{H}}.$$
 (30)

A linear combination of (30) yields (10).

B. Proof of Proposition 1

The scattering matrix of BD-RIS can be decomposed as⁶

$$\mathbf{\Theta} = \mathbf{L}\mathbf{\Theta}_{\mathbf{D}}\mathbf{R}^{\mathsf{H}},\tag{31}$$

where $\Theta_{\rm D} \in \mathbb{U}^{N_{\rm S} \times N_{\rm S}}$ corresponds to diagonal RIS and $\mathbf{L}, \mathbf{R} \in \mathbb{U}^{N_{\rm S} \times N_{\rm S}}$ are block diagonal matrices of $L \times L$ unitary blocks. Manipulating \mathbf{L} and \mathbf{R} rotates the linear spans of $\bar{\mathbf{H}}_{\rm B} \triangleq \mathbf{H}_{\rm B} \mathbf{L}$ and $\bar{\mathbf{H}}_{\rm F} \triangleq \mathbf{R}^{\rm H} \mathbf{H}_{\rm F}$ and maintains their rank. On the other hand, there exists a $\Theta_{\rm D}$ such that

$$\begin{split} \operatorname{rank}(\mathbf{H}_{\mathrm{B}}\mathbf{\Theta}_{\mathrm{D}}\mathbf{H}_{\mathrm{F}}) &= \min \big(\operatorname{rank}(\mathbf{H}_{\mathrm{B}}), \operatorname{rank}(\mathbf{\Theta}_{\mathrm{D}}), \operatorname{rank}(\mathbf{H}_{\mathrm{F}}) \big) \\ &= \min \big(\operatorname{rank}(\bar{\mathbf{H}}_{\mathrm{B}}), N_{\mathrm{S}}, \operatorname{rank}(\bar{\mathbf{H}}_{\mathrm{F}}) \big) \\ &= \max_{\mathbf{\Theta}} \ \operatorname{rank}(\mathbf{H}_{\mathrm{B}}\mathbf{\Theta}\mathbf{H}_{\mathrm{F}}) \end{split}$$

The same result holds if the direct link is present.

C. Proof of Proposition 2

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

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

where we define $\mathbf{Y} \triangleq \mathbf{H}_{\mathrm{D}}(\mathbf{I} - \mathbf{V}_{\mathrm{F}}\mathbf{V}_{\mathrm{F}}^{\mathrm{H}})\mathbf{H}_{\mathrm{D}}^{\mathrm{H}} \in \mathbb{H}^{N_{\mathrm{R}} \times N_{\mathrm{R}}}$ 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 [53], the n-th eigenvalue of \mathbf{G} is bounded by

$$\lambda_n(\mathbf{G}) \le \lambda_{n-k}(\mathbf{Y}), \quad \text{if } n > k,$$
 (32)

$$\lambda_n(\mathbf{G}) \ge \lambda_n(\mathbf{Y}), \quad \text{if } n < N - k + 1.$$
 (33)

Since $Y = TT^H$ is positive semi-definite, taking the square roots of (32) and (33) gives (11) and (12).

D. 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 RIS can be decomposed as

$$\Theta = \mathbf{V}_{\mathbf{B}} \mathbf{X} \mathbf{U}_{\mathbf{F}}^{\mathsf{H}},\tag{34}$$

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}

$$\mathbf{H} = \mathbf{H}_{\mathrm{B}} \mathbf{\Theta} \mathbf{H}_{\mathrm{F}} = \mathbf{U}_{\mathrm{B}} \mathbf{\Sigma}_{\mathrm{B}} \mathbf{X} \mathbf{\Sigma}_{\mathrm{F}} \mathbf{V}_{\mathrm{F}}^{\mathsf{H}}. \tag{35}$$

Since $sv(UAV^H) = sv(A)$ for unitary U and V, we have

$$\begin{split} \mathrm{sv}(\mathbf{H}) &= \mathrm{sv}(\mathbf{U}_{\mathrm{B}} \boldsymbol{\Sigma}_{\mathrm{B}} \mathbf{X} \boldsymbol{\Sigma}_{\mathrm{F}} \mathbf{V}_{\mathrm{F}}^{\mathsf{H}}) \\ &= \mathrm{sv}(\boldsymbol{\Sigma}_{\mathrm{B}} \mathbf{X} \boldsymbol{\Sigma}_{\mathrm{F}}) \\ &= \mathrm{sv}(\bar{\mathbf{U}}_{\mathrm{B}} \boldsymbol{\Sigma}_{\mathrm{B}} \bar{\mathbf{V}}_{\mathrm{B}}^{\mathsf{H}} \bar{\mathbf{U}}_{\mathrm{F}} \boldsymbol{\Sigma}_{\mathrm{F}} \bar{\mathbf{V}}_{\mathrm{F}}^{\mathsf{H}}) \\ &= \mathrm{sv}(\mathbf{B}\mathbf{F}). \end{split}$$

where $\bar{\mathbf{U}}_{\mathrm{B/F}}$ and $\bar{\mathbf{V}}_{\mathrm{B/F}}$ are arbitrary unitary matrices.

E. Proof of Lemma 2

The differential of R w.r.t. Θ_q^* is [55]

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

and the corresponding complex derivative is (22).

F. Proof of Proposition 4

The differential of (24a) w.r.t. Θ_a^* is

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

and the corresponding complex derivative is

$$\frac{\partial \|\mathbf{H}\|_{\mathrm{F}}^{2}}{\partial \mathbf{\Theta}_{a}^{*}} = \mathbf{H}_{\mathrm{B},g}^{\mathsf{H}} (\mathbf{H}_{\mathrm{D}} + \mathbf{H}_{\mathrm{B}} \mathbf{\Theta} \mathbf{H}_{\mathrm{F}}) \mathbf{H}_{\mathrm{F},g}^{\mathsf{H}} = \mathbf{M}_{g}.$$
(36)

First, we approximate the quadratic objective (24a) by its local Taylor expansion

$$\max_{\mathbf{\Theta}} \quad \sum_{g} 2\Re \left\{ \operatorname{tr}(\mathbf{\Theta}_{g}^{\mathsf{H}} \mathbf{M}_{g}) \right\} \tag{37a}$$

s.t.
$$\Theta_q^{\mathsf{H}}\Theta_g = \mathbf{I}, \quad \forall g.$$
 (37b)

Let $\mathbf{M}_g = \mathbf{U}_g \mathbf{\Sigma}_g \mathbf{V}_g^{\mathsf{H}}$ be the compact SVD of \mathbf{M}_g . We have

$$\Re \left\{ \operatorname{tr}(\boldsymbol{\Theta}_g^{\mathsf{H}} \mathbf{M}_g) \right\} = \Re \left\{ \operatorname{tr}(\boldsymbol{\Sigma}_g \mathbf{V}_g^{\mathsf{H}} \boldsymbol{\Theta}_g^{\mathsf{H}} \mathbf{U}_g) \right\} \le \operatorname{tr}(\boldsymbol{\Sigma}_g). \tag{38}$$

The upper bound is tight when $\mathbf{V}_g^H \mathbf{\Theta}_g^H \mathbf{U}_g = \mathbf{I}$, which implies the optimal solution of (37) is $\tilde{\mathbf{\Theta}}_g = \mathbf{U}_g \mathbf{V}_g^H$, $\forall g$.

Next, we prove that solving (37) successively does not decrease (24a). Since $\tilde{\Theta}$ optimal for problem (37), we have $\sum_g 2\Re\{\mathrm{tr}(\tilde{\Theta}_g^\mathsf{H}\mathbf{M}_g)\} \geq \sum_g 2\Re\{\mathrm{tr}(\Theta_g^\mathsf{H}\mathbf{M}_g)\}$ which is explicitly expressed by (40). On the other hand, expanding

⁶This is because (block) unitary matrices are closed under multiplication.

$$2\Re\left\{\sum_{g} \mathrm{tr}(\tilde{\mathbf{\Theta}}_{g}^{\mathsf{H}}\mathbf{H}_{\mathrm{B},g}^{\mathsf{H}}\mathbf{H}_{\mathrm{D}}\mathbf{H}_{\mathrm{F},g}^{\mathsf{H}}) + \sum_{g_{1},g_{2}} \mathrm{tr}(\tilde{\mathbf{\Theta}}_{g_{1}}^{\mathsf{H}}\mathbf{H}_{\mathrm{B},g_{2}}^{\mathsf{H}}\mathbf{\Theta}_{g_{2}}\mathbf{H}_{\mathrm{F},g_{2}}\mathbf{H}_{\mathrm{F},g_{1}}^{\mathsf{H}})\right\} \geq 2\Re\left\{\sum_{g} \mathrm{tr}(\mathbf{\Theta}_{g}^{\mathsf{H}}\mathbf{H}_{\mathrm{B},g}^{\mathsf{H}}\mathbf{H}_{\mathrm{D}}\mathbf{H}_{\mathrm{F},g}^{\mathsf{H}}) + \sum_{g_{1},g_{2}} \mathrm{tr}(\mathbf{\Theta}_{g_{1}}^{\mathsf{H}}\mathbf{H}_{\mathrm{B},g_{2}}^{\mathsf{H}}\mathbf{\Theta}_{g_{2}}\mathbf{H}_{\mathrm{F},g_{2}}\mathbf{H}_{\mathrm{F},g_{1}}^{\mathsf{H}})\right\} \quad (40)$$

$$\sum_{g_1,g_2} \operatorname{tr}(\mathbf{H}_{F,g_1}^{\mathsf{H}} \tilde{\mathbf{\Theta}}_{g_1}^{\mathsf{H}} \mathbf{H}_{B,g_1}^{\mathsf{H}} \mathbf{H}_{B,g_2} \tilde{\mathbf{\Theta}}_{g_2} \mathbf{H}_{F,g_2}) - 2\Re \left\{ \sum_{g_1,g_2} \operatorname{tr}(\mathbf{H}_{F,g_1}^{\mathsf{H}} \tilde{\mathbf{\Theta}}_{g_1}^{\mathsf{H}} \mathbf{H}_{B,g_1}^{\mathsf{H}} \mathbf{H}_{B,g_2} \mathbf{\Theta}_{g_2} \mathbf{H}_{F,g_2}) \right\} + \sum_{g_1,g_2} \operatorname{tr}(\mathbf{H}_{F,g_1}^{\mathsf{H}} \tilde{\mathbf{\Theta}}_{g_1}^{\mathsf{H}} \mathbf{H}_{B,g_2} \mathbf{\Theta}_{g_2} \mathbf{H}_{F,g_2}) \ge 0 \quad (41)$$

 $\|\sum_g \mathbf{H}_{\mathrm{B},g} \tilde{\mathbf{\Theta}}_g \mathbf{H}_{\mathrm{F},g} - \sum_g \mathbf{H}_{\mathrm{B},g} \mathbf{\Theta}_g \mathbf{H}_{\mathrm{F},g}\|_{\mathrm{F}}^2 \ge 0$ gives (41). [12] Y. Zhao, B. Clerckx, and Z. Feng, "Irs-aided swipt: Joint waveform, active and passive beamforming design under nonlinear harvester model."

$$\begin{split} &2\Re\!\left\{\mathrm{tr}(\tilde{\boldsymbol{\Theta}}^{\mathsf{H}}\mathbf{H}_{\mathrm{B}}^{\mathsf{H}}\mathbf{H}_{\mathrm{D}}\mathbf{H}_{\mathrm{F}}^{\mathsf{H}})\right\}\!+\!\mathrm{tr}(\mathbf{H}_{\mathrm{F}}^{\mathsf{H}}\tilde{\boldsymbol{\Theta}}^{\mathsf{H}}\mathbf{H}_{\mathrm{B}}^{\mathsf{H}}\mathbf{H}_{\mathrm{B}}\tilde{\boldsymbol{\Theta}}\mathbf{H}_{\mathrm{F}})\\ &\geq\!2\Re\!\left\{\mathrm{tr}(\boldsymbol{\Theta}^{\mathsf{H}}\mathbf{H}_{\mathrm{B}}^{\mathsf{H}}\mathbf{H}_{\mathrm{D}}\mathbf{H}_{\mathrm{F}}^{\mathsf{H}})\right\}\!+\!\mathrm{tr}(\mathbf{H}_{\mathrm{F}}^{\mathsf{H}}\boldsymbol{\Theta}^{\mathsf{H}}\mathbf{H}_{\mathrm{B}}^{\mathsf{H}}\mathbf{H}_{\mathrm{B}}\boldsymbol{\Theta}\mathbf{H}_{\mathrm{F}}),\quad(39)\end{split}$$

which suggests that updating $\tilde{\Theta}$ does not decrease (24a).

Finally, we prove that the converging point of (37), denoted by $\Theta^{?}$, is a stationary point of (24). The Karush-Kuhn-Tucker (KKT) conditions of (24) and (37) are equivalent in terms of primal/dual feasibility and complementary slackness, while the stationary conditions are respectively, $\forall q$,

$$\mathbf{H}_{\mathrm{B},g}^{\mathsf{H}}(\mathbf{H}_{\mathrm{D}} + \mathbf{H}_{\mathrm{B}}\boldsymbol{\Theta}^{\star}\mathbf{H}_{\mathrm{F}})\mathbf{H}_{\mathrm{F},g}^{\mathsf{H}} - \boldsymbol{\Theta}_{g}^{\star}\boldsymbol{\Lambda}_{g}^{\mathsf{H}} = 0, \qquad (42)$$
$$\mathbf{M}_{q} - \boldsymbol{\Theta}_{q}^{\star}\boldsymbol{\Lambda}_{q}^{\mathsf{H}} = 0. \qquad (43)$$

On convergence, (43) becomes $\mathbf{H}_{\mathrm{B},g}^{\mathsf{H}}(\mathbf{H}_{\mathrm{D}}+\mathbf{H}_{\mathrm{B}}\boldsymbol{\Theta}^{?}\mathbf{H}_{\mathrm{F}})\mathbf{H}_{\mathrm{F},g}^{\mathsf{H}}-\boldsymbol{\Theta}_{g}^{?}\boldsymbol{\Lambda}_{g}^{\mathsf{H}}=0$ and reduces to (42). The proof is thus completed.

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