

## I. SYSTEM MODEL

Consider an IRS-aided multiuser SISO SWIPT system where the IRS not only assists the primal transmission but also retrieves Channel State Information (CSI) and harvests energy for its own operation. The single-antenna transmitter delivers information and power simultaneously, through the  $L$ -reflector IRS, to  $K$  single-antenna users over  $N$  orthogonal subbands. Assume a total bandwidth  $B$  and evenly-spaced carriers around center frequency  $f_0$ . Denote the frequency of the  $n$ -th subband as  $f_n$  ( $n = 1, \dots, N$ ). It is assumed that the IRS performs channel estimation in the first subframe and supports information and power transfer in the second subframe [1]. Due to the passive characteristics of IRS, we consider a Time-Division Duplexing (TDD) protocol where the CSI can be obtained by exploiting channel reciprocity. Perfect CSI is assumed at the AP and IRS to investigate the analytical upper-bound of the proposed system. A quasi-static frequency-selective model is used for both the AP-user and AP-IRS-user links where the channels are assumed unchanged within each transmission frame. The signals reflected by IRS for two and more times are assumed negligible and thus not considered. Note that although Frequency Selective Surface (FSS) has received much attention for wideband communications, active FSS requires RF-chains thus becomes prohibitive in IRS [2], [3]. Since passive FSS is not reconfigurable with fixed physical characteristics [4], we assume a frequency-flat IRS with the same reflection coefficients for all subbands. Since a deterministic multisine waveform can boost the energy transfer efficiency [5] and creates no interference to the information signal [6], we use a superposition of multicarrier modulated and unmodulated waveforms, both transmitted on the same frequency bands, to maximize the rate-energy tradeoff. Two practical receiver architectures proposed in [7], namely Time Switching (TS) and Power Splitting (PS), are investigated for the co-located information decoder and energy harvester. In the TS strategy, each transmission subframe is further divided into orthogonal data and energy slots, with duration ratio  $(1 - \alpha)$  and  $\alpha$  respectively. Hence, the achievable rate-energy region can be obtained through a time sharing between wireless power transfer (WPT) with  $\alpha = 1$  and wireless information transfer (WIT) with  $\alpha = 0$ . The adjustment of  $\alpha$  has no impact on the transmit waveform and IRS elements design as they are optimized individually in data and energy slots. In comparison, the PS scheme splits the received signal into data and energy streams with power ratio  $(1 - \rho)$  and  $\rho$  such that the PS ratio is coupled with waveform design. Perfect synchronization is assumed among the three parties in both scenarios.

### A. Transmit Signal

1) *Modulated Information Waveform:* Let  $\tilde{x}_{I,k,n}$  be the information symbol of user  $k$  ( $k = 1, \dots, K$ ) over subband  $n$ , which follows a capacity-achieving i.i.d. Circular Symmetric Complex Gaussian (CSCG) distribution  $\tilde{x}_{I,k,n} \sim \mathcal{CN}(0, 1)$ . The transmit information signal at time  $t$  is

$$x_I(t) = \Re \left\{ \sum_{k=1}^K \sum_{n=1}^N w_{I,k,n} \tilde{x}_{I,k,n}(t) e^{j2\pi f_n t} \right\} \quad (1)$$

where  $w_{I,k,n} = s_{I,k,n} e^{j\phi_{I,k,n}}$  collects the magnitude and phase of the information signal of user  $k$  at frequency  $n$ . We further define the information waveform vector  $\mathbf{w}_{I,k} = [w_{I,k,1}, \dots, w_{I,k,N}]^T \in \mathbb{C}^{N \times 1}$ .

2) *Unmodulated Power Waveform:* With no randomness over time, the transmit power signal is

$$x_P = \Re \left\{ \sum_{k=1}^K \sum_{n=1}^N w_{P,k,n} e^{j2\pi f_n t} \right\} = \Re \left\{ \sum_{n=1}^N w_{P,n} e^{j2\pi f_n t} \right\} \quad (2)$$

where  $w_{P,n} = s_{P,n} e^{j\phi_{P,n}} = \sum_{k=1}^K w_{P,k,n}$  combines the magnitude and phase on the  $n$ -th power tone over all users. Also, collect  $w_{P,n}$  into power waveform vector  $\mathbf{w}_P = [w_{P,1}, \dots, w_{P,N}]^T \in \mathbb{C}^{N \times 1}$ .

Therefore, the superposed transmit signal at time  $t$  over subband  $n$  is

$$x(t) = \Re \left\{ \sum_{n=1}^N \left( \sum_{k=1}^K w_{I,k,n} \tilde{x}_{I,k,n}(t) + w_{P,n} \right) e^{j2\pi f_n t} \right\} \quad (3)$$

### B. Composite Channel Model

Denote the frequency response of the AP-user  $k$  direct link as  $\mathbf{h}_{D,k} = [h_{D,k,1}, \dots, h_{D,k,N}]^T \in \mathbb{C}^{N \times 1}$ . Let  $[\mathbf{h}_{I,1}, \dots, \mathbf{h}_{I,N}] \in \mathbb{C}^{L \times N}$  be the frequency response of AP-IRS incident channel, where  $\mathbf{h}_{I,n} \in \mathbb{C}^{L \times 1}$  corresponds to the  $n$ -th incident channel. Similarly, let  $[\mathbf{h}_{R,k,1}, \dots, \mathbf{h}_{R,k,N}]^H \in \mathbb{C}^{N \times L}$  be the frequency response of IRS-user  $k$  reflective channel, where  $\mathbf{h}_{R,k,n}^H \in \mathbb{C}^{1 \times L}$  corresponds to the  $n$ -th reflective channel. At the IRS, element  $l$  ( $l = 1, \dots, L$ ) redistributes the received signal by adjusting the amplitude reflection coefficient  $\beta_l \in [0, 1]$  and phase shift  $\theta_l \in [0, 2\pi)$ <sup>1</sup>. On top of this, the IRS matrix is constructed by collecting the reflection coefficients onto the main diagonal entries as  $\mathbf{\Theta} = \text{diag} \{ \beta_1 e^{j\theta_1}, \dots, \beta_L e^{j\theta_L} \} \in \mathbb{C}^{L \times L}$ . The IRS-aided link can be modeled as a concatenation of the AP-IRS channel, IRS reflection, and IRS-user  $k$  channel, which for user  $k$  over subband  $n$  is

$$h_{E,k,n} = \mathbf{h}_{R,k,n}^H \mathbf{\Theta} \mathbf{h}_{I,n} = \mathbf{v}_{k,n}^H \boldsymbol{\phi} \quad (4)$$

where  $\mathbf{v}_{k,n}^H \triangleq \mathbf{h}_{R,k,n}^H \text{diag}(\mathbf{h}_{I,n}) \in \mathbb{C}^{1 \times L}$  and  $\boldsymbol{\phi} = [e^{j\theta_1}, \dots, e^{j\theta_L}] \in \mathbb{C}^{L \times 1}$ . Both direct and extra link contributes to the corresponding composite channel as

$$h_{k,n} = h_{D,k,n} + \mathbf{v}_{k,n}^H \boldsymbol{\phi} \quad (5)$$

Let  $\mathbf{V}_k^H = [\mathbf{v}_{k,1}, \dots, \mathbf{v}_{k,N}]^H \in \mathbb{C}^{N \times L}$ , the extra link for user  $k$  is  $\mathbf{h}_{E,k} = [h_{E,k,1}, \dots, h_{E,k,N}]^T = \mathbf{V}_k^H \boldsymbol{\phi} \in \mathbb{C}^{N \times 1}$ . Therefore, the composite channel of user  $k$  is

$$\mathbf{h}_k = \mathbf{h}_D + \mathbf{V}_k^H \boldsymbol{\phi} \quad (6)$$

<sup>1</sup>To investigate the performance upper bound of IRS, we suppose the reflection coefficient is maximized  $\beta_l = 1 \ \forall l$  while the phase shift is a continuous variable over  $[0, 2\pi)$ .

### C. Receive Signal

The RF signal received by user  $k$  captures the contribution of information and power waveforms through both direct and reflective links as

$$y_k(t) = \Re \left\{ \sum_{n=1}^N h_{k,n} \left( \sum_{j=1}^K w_{I,j,n} \tilde{x}_{I,j,n}(t) + w_{P,n} \right) e^{j2\pi f_n t} \right\} \quad (7)$$

which can be divided into

$$y_{I,k}(t) = \Re \left\{ \sum_{j=1}^K \sum_{n=1}^N h_{k,n} w_{I,j,n} \tilde{x}_{I,j,n}(t) e^{j2\pi f_n t} \right\} \quad (8)$$

$$y_{P,k}(t) = \Re \left\{ \sum_{n=1}^N h_{k,n} w_{P,n} e^{j2\pi f_n t} \right\} \quad (9)$$

### D. Information Decoder

One major benefit of the superposed waveform is that the power component  $y_{P,k}(t)$  creates no interference to the information component  $y_{I,k}(t)$ . Hence, the achievable rate of user  $k$  is

$$R_k(\{\mathbf{w}_{I,k}\}, \phi, \rho) = \sum_{n=1}^N \log_2 \left( 1 + \frac{(1-\rho)|h_{k,n}w_{I,k,n}|^2}{\sigma_n^2} \right) \quad (10)$$

where  $\sigma_n^2$  is the variance of the noise at RF band and during RF-to-BB conversion on tone  $n$ . Rate 10 is achievable with either waveform cancellation or translated demodulation [6].

### E. Energy Harvester

Consider a nonlinear diode model based on the Taylor expansion of a small signal model [5], [6], which highlights the dependency of harvester output DC current on the received waveform of user  $k$  as

$$i_k(\{\mathbf{w}_{I,k}\}, \{\mathbf{w}_{P,k}\}, \phi, \rho) \approx \sum_{i=0}^{\infty} k'_i \rho^{i/2} R_{\text{ant}}^{i/2} \mathcal{E} \{ \mathcal{A} \{ y_k(t)^i \} \} \quad (11)$$

where  $R_{\text{ant}}$  is the impedance of the receive antenna,  $k'_0 = i_s(e^{-i_k R_{\text{ant}}/nv_t} - 1)$ ,  $k'_i = i_s e^{-i_k R_{\text{ant}}/nv_t} / i! (nv_t)^i$  for  $i = 1, \dots, \infty$ ,  $i_s$  is saturation current,  $n$  is diode ideality factor,  $v_t$  is thermal voltage. For a fixed channel and waveform,  $\mathcal{A} \{ \cdot \}$  extracts the DC component of the received signal while  $\mathcal{E} \{ \cdot \}$  covers the expectation over  $\tilde{x}_{I,k,n}$ .

With the assumption of evenly spaced frequencies, we have  $\mathcal{E} \{ y_k(t)^i \} = 0 \forall i$  odd such that the related terms has no contribution to DC components. For simplicity, we truncate the infinite series to the  $n_0$ -th order. Maximizing a truncated 11 is equivalent to maximizing a monotonic function [5]

$$z_k(\{\mathbf{w}_{I,k}\}, \{\mathbf{w}_{P,k}\}, \phi, \rho) = \sum_{i \text{ even}, i \geq 2}^{n_0} k_i \rho^{i/2} R_{\text{ant}}^{i/2} \mathcal{E} \{ \mathcal{A} \{ y_k(t)^i \} \} \quad (12)$$

where  $k_i = i_s / i! (nv_t)^i$ . We choose  $n_0 = 4$  to investigate the fundamental impact of diode nonlinearity on energy harvest. Nonzero terms are given in 13 – 17. Note that  $\mathcal{E} \{ |\tilde{x}_{k,n}|^2 \} = 1$

and  $\mathcal{E} \{ |\tilde{x}_{k,n}|^4 \} = 2$ , which can be interpreted as a modulation gain in the nonlinear terms of the output DC current. On top of this, the current expression 12 reduces to 18.

## II. PROBLEM FORMULATION

In this section, we first define the weighted sum rate-energy (WSR-E) region then formulate waveform and IRS optimization problems.

### A. Weighted Sum Rate-Energy Region

We define the achievable WSR-E region as

$$C_{R-I}(P) \triangleq \left\{ (R, I) : R \leq \sum_{k=1}^K u_{I,k} R_k, I \leq \sum_{k=1}^K u_{P,k} z_k, \right. \\ \left. \frac{1}{2}(\mathbf{w}_I^H \mathbf{w}_I + \mathbf{w}_P^H \mathbf{w}_P) \leq P \right\} \quad (19)$$

where  $u_{I,k}, u_{P,k}$  denote the information and power weight of user  $k$ .

### B. Single-User Optimization

In this section, we first characterize the rate-energy region in the single-user setup. Let  $h_n = A_n e^{j\psi_n}$ ,  $w_{I,n} = s_{I,n} e^{j\phi_n}$ ,  $w_{P,n} = s_{P,n} e^{j\phi_n}$ . The WSR-E region can be obtained through a rate maximization problem subject to transmit power and output DC current constraints

$$\mathbf{w}_I, \mathbf{w}_P, \mathbf{v}, \rho \quad \sum_n \log_2 \left( 1 + \frac{(1-\rho)|h_{D,n} + \Phi_n^H \mathbf{v}|^2}{\sigma_n^2} \right) \\ \text{s.t.} \quad \frac{1}{2}(\mathbf{w}_I^H \mathbf{w}_I + \mathbf{w}_P^H \mathbf{w}_P) \leq P, \\ z(\mathbf{w}_I, \mathbf{w}_P, \mathbf{v}, \rho) \geq \bar{z}, \\ |\mathbf{v}_l| = 1, \quad l = 1, \dots, L \quad (20)$$

Problem 20 is intricate due to the non-convex rate function, unit-modulus constraint, and non-convex DC current requirement with coupled variables.

1) *Frequency-Selective IRS*: In frequency-selective IRS, each element is expected to provide adjustable subband-dependent reflection coefficients such that the total degree of freedom (DoF) of IRS is  $NL$ . Therefore,  $\mathbf{v}_n$  replaces  $\mathbf{v}$  in 20. Note that  $|(h_{D,n} + \Phi_n^H \mathbf{v}_n)w_{I,n}| \leq |h_{D,n}w_{I,n}| + |\Phi_n^H \mathbf{v}_n w_{I,n}|$  where the equality holds if and only if the direct and IRS-aided links are aligned by

$$\theta_{n,l}^* = \angle h_{D,n} - \angle h_{R,n,l} - \angle h_{I,n,l} \quad (21)$$

That is to say, the optimal phase shift is obtained in closed form in the single-user scenario. On top of this, it can be observed from ??, 10 and 18 that the optimal phase of information and power waveforms are matched to composite frequency response as

$$\phi_{I,n}^* = \phi_{P,n}^* = -\bar{\psi}_n \quad (22)$$

With all the phases determined, the original problem 20 is equivalent to reduced to

$$\begin{aligned} \max_{\mathbf{s}_I, \mathbf{s}_P, \rho} \quad & \sum_n \log_2 \left( 1 + \frac{(1-\rho)A_n^2 s_{I,n}^2}{\sigma_n^2} \right) \\ \text{s.t.} \quad & \frac{1}{2}(\mathbf{s}_I^H \mathbf{s}_I + \mathbf{s}_P^H \mathbf{s}_P) \leq P, \\ & z(\mathbf{s}_I, \mathbf{s}_P, \rho) \geq \bar{z} \end{aligned} \quad (23)$$

with  $z$  given by 24. It can be transformed to an equivalent problem by introducing an auxiliary variable  $t_0$

$$\begin{aligned} \min_{\mathbf{s}_I, \mathbf{s}_P, \rho} \quad & \frac{1}{t_0} \\ \text{s.t.} \quad & \frac{1}{2}(\mathbf{s}_I^H \mathbf{s}_I + \mathbf{s}_P^H \mathbf{s}_P) \leq P, \\ & \frac{t_0}{\prod_n \left( 1 + \frac{(1-\rho)A_n^2 s_{I,n}^2}{\sigma_n^2} \right)} \leq 1, \\ & \frac{\bar{z}}{z(\mathbf{s}_I, \mathbf{s}_P, \rho)} \leq 1 \end{aligned} \quad (25)$$

$$\begin{aligned} \min_{\mathbf{s}_I, \mathbf{s}_P, \rho} \quad & \frac{1}{t_0} \\ \text{s.t.} \quad & \frac{1}{2}(\mathbf{s}_I^H \mathbf{s}_I + \mathbf{s}_P^H \mathbf{s}_P) \leq P, \\ & t_0 \prod_n \left( \frac{1}{\gamma_{I,n,1}} \right)^{-\gamma_{I,n,1}} \left( \frac{\bar{\rho} A_n^2 s_{I,n}^2}{\sigma_n^2 \gamma_{I,n,2}} \right)^{-\gamma_{I,n,2}} \leq 1, \\ & \bar{z} \prod_{m_P} \left( \frac{g_{P,m_P}(\mathbf{s}_I, \mathbf{s}_P, \rho)}{\gamma_{P,m_P}} \right)^{-\gamma_{P,m_P}} \leq 1, \\ & \rho + \bar{\rho} \leq 1 \end{aligned} \quad (26)$$

25 is a Reversed Geometric Program which can be transformed to standard Geometric Program (GP). The basic idea is to decompose the information and power posynomials as sum of monomials, then derive their upper bounds using Arithmetic Mean-Geometric Mean (AM-GM) inequality [6], [8]. Let  $z(\mathbf{s}_I, \mathbf{s}_P, \rho) = \sum_{m_P=1}^{M_P} g_{P,m_P}(\mathbf{s}_I, \mathbf{s}_P, \rho)$ , problem 25 is

where  $\gamma_{I,n,1}, \gamma_{I,n,2} \geq 0$ ,  $\gamma_{I,n,1} + \gamma_{I,n,2} = 1$ ,  $\gamma_{P,m_P} \geq 0, \forall m_P = 1, \dots, M_P$  and  $\sum_{m_P=1}^{M_P} \gamma_{P,m_P} = 1$ . As suggested in [6], the tightness of the AM-GM inequality depends on  $\{\gamma_{I,n}, \gamma_P\}$  that require iterative update. At iteration  $i$ , we

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$$\mathcal{E}\{\mathcal{A}\{y_{I,k}^2(t)\}\} = \frac{1}{2} \sum_{j_1, j_2} \sum_n (h_{k,n} w_{I,j_1,n}) (h_{k,n} w_{I,j_2,n})^* = \frac{1}{2} \sum_n h_{k,n} h_{k,n}^* \mathbf{w}_{I,n}^H \mathbf{J}_K \mathbf{w}_{I,n} \quad (13)$$

$$\begin{aligned} \mathcal{E}\{\mathcal{A}\{y_{I,k}^4(t)\}\} &= \frac{3}{4} \sum_{j_1, j_2, j_3, j_4} \sum_{\substack{n_1, n_2, n_3, n_4 \\ n_1 + n_2 = n_3 + n_4}} (h_{k,n_1} w_{I,j_1,n_1}) (h_{k,n_2} w_{I,j_2,n_2}) (h_{k,n_3} w_{I,j_3,n_3})^* (h_{k,n_4} w_{I,j_4,n_4})^* \\ &= \frac{3}{4} \sum_{\substack{n_1, n_2, n_3, n_4 \\ n_1 + n_2 = n_3 + n_4}} h_{k,n_3}^* h_{k,n_1} h_{k,n_4}^* h_{k,n_2} (\mathbf{w}_{I,n_3}^H \mathbf{J}_K \mathbf{w}_{I,n_1}) (\mathbf{w}_{I,n_4}^H \mathbf{J}_K \mathbf{w}_{I,n_2}) \end{aligned} \quad (14)$$

$$\mathcal{A}\{y_{P,k}^2(t)\} = \frac{1}{2} \sum_n (h_{k,n} w_{P,n}) (h_{k,n} w_{P,n})^* \quad (15)$$

$$\mathcal{A}\{y_{P,k}^4(t)\} = \frac{3}{8} \sum_{\substack{n_1, n_2, n_3, n_4 \\ n_1 + n_2 = n_3 + n_4}} (h_{k,n_1} w_{P,n_1}) (h_{k,n_2} w_{P,n_2}) (h_{k,n_3} w_{P,n_3})^* (h_{k,n_4} w_{P,n_4})^* \quad (16)$$

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$$\begin{aligned} z_k &= k_2 \rho R_{\text{ant}} (\mathcal{E}\{\mathcal{A}\{y_{I,k}^2(t)\}\} + \mathcal{A}\{y_{P,k}^2(t)\}) + k_4 \rho^2 R_{\text{ant}}^2 (\mathcal{E}\{\mathcal{A}\{y_{I,k}^4(t)\}\} + \mathcal{A}\{y_{P,k}^4(t)\}) + 6 \mathcal{E}\{\mathcal{A}\{y_{I,k}^2(t)\}\} \mathcal{A}\{y_{P,k}^2(t)\}) \\ &= \frac{1}{2} k_2 \rho R_{\text{ant}} \sum_n h_{k,n} h_{k,n}^* (\mathbf{w}_{I,n}^H \mathbf{J}_K \mathbf{w}_{I,n} + \mathbf{w}_{P,n}^H \mathbf{J}_K \mathbf{w}_{P,n}) \\ &\quad + \frac{3}{8} k_4 \rho^2 R_{\text{ant}}^2 \sum_{\substack{n_1, n_2, n_3, n_4 \\ n_1 + n_2 = n_3 + n_4}} h_{k,n_3}^* h_{k,n_1} h_{k,n_4}^* h_{k,n_2} (2(\mathbf{w}_{I,n_3}^H \mathbf{J}_K \mathbf{w}_{I,n_1}) (\mathbf{w}_{I,n_4}^H \mathbf{J}_K \mathbf{w}_{I,n_2}) + (\mathbf{w}_{P,n_3}^H \mathbf{J}_K \mathbf{w}_{P,n_1}) (\mathbf{w}_{P,n_4}^H \mathbf{J}_K \mathbf{w}_{P,n_2})) \\ &\quad + \frac{3}{2} k_4 \rho^2 R_{\text{ant}}^2 \sum_n h_{k,n}^2 h_{k,n}^* (\mathbf{w}_{I,n}^H \mathbf{J}_K \mathbf{w}_{I,n}) (\mathbf{w}_{P,n}^H \mathbf{J}_K \mathbf{w}_{P,n}) \end{aligned} \quad (17)$$

choose

$$\gamma_{I,n,1}^{(i)} = \frac{1}{1 + \frac{\bar{\rho}^{(i-1)} A_n^2 s_{I,n}^{(i-1)2}}{\sigma_n^2}}, \quad n = 1, \dots, N, \quad (27)$$

$$\gamma_{I,n,2}^{(i)} = \frac{\frac{\bar{\rho}^{(i-1)} A_n^2 s_{I,n}^{(i-1)2}}{\sigma_n^2}}{1 + \frac{\bar{\rho}^{(i-1)} A_n^2 s_{I,n}^{(i-1)2}}{\sigma_n^2}}, \quad n = 1, \dots, N, \quad (28)$$

$$\gamma_{P,m_P}^{(i)} = \frac{g_{P,m_P}(\mathbf{s}_I^{(i-1)}, \mathbf{s}_P^{(i-1)}, \rho^{(i-1)})}{z(\mathbf{s}_I^{(i-1)}, \mathbf{s}_P^{(i-1)}, \rho^{(i-1)})}, \quad m_P = 1, \dots, M_P \quad (29)$$

and then solve problem 26.

2) *Frequency-Flat IRS*: In contrast, frequency-flat IRS reflects all subbands equally with a DoF of  $L$ . We observe that

$$\begin{aligned} |h_{D,n} + \Phi_n^H \mathbf{v}|^2 &= |h_{D,n}|^2 + h_{D,n}^* \Phi_n^H \mathbf{v} + \mathbf{v}^H \Phi_n h_{D,n} + \mathbf{v}^H \Phi_n \Phi_n^H \mathbf{v} \\ &= \bar{\mathbf{v}}^H \mathbf{R} \bar{\mathbf{v}} = \text{Tr}(\mathbf{R}_n \bar{\mathbf{v}} \bar{\mathbf{v}}^H) = \text{Tr}(\mathbf{R}_n \mathbf{V}) \end{aligned} \quad (30)$$

where  $t$  is an auxiliary variable with unit modulus and

$$\mathbf{R}_n = \begin{bmatrix} \Phi_n \Phi_n^H & \Phi_n h_{D,n} \\ h_{D,n}^* \Phi_n^H & h_{D,n}^* h_{D,n} \end{bmatrix}, \quad \bar{\mathbf{v}} = \begin{bmatrix} \mathbf{v} \\ t \end{bmatrix}, \quad \bar{\mathbf{V}} = \bar{\mathbf{v}} \bar{\mathbf{v}}^H \quad (31)$$

Hence, 20 is transformed to

$$\begin{aligned} \max_{\mathbf{w}_I, \mathbf{w}_P, \mathbf{V}, \rho} \quad & \sum_n \log_2 \left( 1 + \frac{(1-\rho)|w_{I,n}|^2 \text{Tr}(\mathbf{R}_n \mathbf{V})}{\sigma_n^2} \right) \\ \text{s.t.} \quad & \frac{1}{2}(\mathbf{w}_I^H \mathbf{w}_I + \mathbf{w}_P^H \mathbf{w}_P) \leq P, \\ & z(\mathbf{w}_I, \mathbf{w}_P, \mathbf{V}, \rho) \geq \bar{z}, \\ & \mathbf{V}_{l,l} = 1, l = 1, \dots, L+1, \\ & \mathbf{V} \succeq 0, \\ & \text{rank}(\mathbf{V}) = 1 \end{aligned} \quad (32)$$

To reduce the design complexity, we propose an suboptimal alternating optimization algorithm that iteratively updates the phase shifts and the waveforms with the other being fixed.

The phase optimization subproblem is formed as follows.

For a given waveform  $\mathbf{w}_I, \mathbf{w}_P, \rho$ , problem 32 reduces to

$$\begin{aligned} \max_{\mathbf{V}} \quad & \sum_n \log_2 \left( 1 + \frac{(1-\rho)|w_{I,n}|^2 \text{Tr}(\mathbf{R}_n \mathbf{V})}{\sigma_n^2} \right) \\ \text{s.t.} \quad & z(\mathbf{V}) \geq \bar{z}, \\ & \mathbf{V}_{l,l} = 1, l = 1, \dots, L+1, \\ & \mathbf{V} \succeq 0, \\ & \text{rank}(\mathbf{V}) = 1 \end{aligned} \quad (33)$$

To tackle the non-convex current constraint, we collect the channel matrices into  $\Phi^H = [\Phi_1, \dots, \Phi_N]^H \in \mathbb{C}^{N \times L}$  and  $\mathbf{h} = \mathbf{h}_D + \Phi^H \mathbf{v} \in \mathbb{C}^{N \times 1}$ . The fixed waveform matrices are defined as  $\mathbf{M}_{I/P} = \mathbf{w}_{I/P}^* \mathbf{w}_{I/P}^T$ . On top of this, let  $\mathbf{M}_{I/P,n}$  keep the  $n$ -th ( $n = -N+1, \dots, N-1$ ) diagonal of  $\mathbf{M}_{I/P}$  and null the remaining entries. Due to the positive definiteness of  $\mathbf{M}_{I/P}$ , we have  $\mathbf{M}_{I/P,-n} = \mathbf{M}_{I/P,n}^H$ . Hence, the output current expression 18 is transformed to 34. We further simplify it by introducing auxiliary variables

$$\begin{aligned} t_{I/P,n} &= \mathbf{h}^H \mathbf{M}_{I/P,n} \mathbf{h} \\ &= \text{Tr}(\mathbf{h} \mathbf{h}^H \mathbf{M}_{I/P,n}) \\ &= \text{Tr}(\mathbf{R}^H \mathbf{V} \mathbf{R} \mathbf{M}_{I/P,n}) \\ &= \text{Tr}(\mathbf{R} \mathbf{M}_{I/P,n} \mathbf{R}^H \mathbf{V}) \\ &= \text{Tr}(\mathbf{C}_{I/P,n} \mathbf{V}) \end{aligned} \quad (35)$$

where  $\mathbf{R}^H = [\Phi^H, \mathbf{h}_D] \in \mathbb{C}^{N \times (L+1)}$  and  $\mathbf{C}_{I/P,n} = \mathbf{R} \mathbf{M}_{I/P,n} \mathbf{R}^H \in \mathbb{C}^{(L+1) \times (L+1)}$ . Therefore, 34 rewrites as

$$\begin{aligned} z &= \frac{1}{2} k_2 \rho R_{\text{ant}} (t_{I,0} + t_{P,0}) \\ &+ \frac{3}{8} k_4 \rho^2 R_{\text{ant}}^2 \sum_{n=-N+1}^{N-1} 2t_{I,n} t_{I,n}^* + t_{P,n} t_{P,n}^* \\ &+ \frac{3}{2} k_4 \rho^2 R_{\text{ant}}^2 t_{I,0} t_{P,0} \end{aligned} \quad (36)$$

We use first-order Taylor expansion to approximate the second-order terms in 36. Based on the variables optimized at iteration  $k-1$ , the local approximations at iteration  $k$  are [9]

$$\begin{aligned} t_{I/P,n}^{(k)} (t_{I/P,n}^{(k)})^* &\approx 2\Re \left\{ t_{I/P,n}^{(k)} (t_{I/P,n}^{(k-1)})^* \right\} - t_{I/P,n}^{(k-1)} (t_{I/P,n}^{(k-1)})^* \\ &= 2\Re \left\{ \text{Tr} \left( (t_{I/P,n}^{(k-1)})^* \mathbf{C}_{I/P,n} \mathbf{V}^{(k)} \right) \right\} - t_{I/P,n}^{(k-1)} (t_{I/P,n}^{(k-1)})^* \\ &= \text{Tr} \left( (t_{I/P,n}^{(k-1)})^* \mathbf{C}_{I/P,n} \mathbf{V}^{(k)} \right) + \text{Tr} (t_{I/P,n}^{(k-1)} \mathbf{C}_{I/P,n}^H \mathbf{V}^{(k)}) \\ &\quad - t_{I/P,n}^{(k-1)} (t_{I/P,n}^{(k-1)})^* \end{aligned} \quad (37)$$

$$\begin{aligned} z &= \frac{1}{2} k_2 \rho R_{\text{ant}} \sum_n A_n^2 (s_{I,n}^2 + s_{P,n}^2) + \frac{3}{8} k_4 \rho^2 R_{\text{ant}}^2 \sum_{\substack{n_1, n_2, n_3, n_4 \\ n_1 + n_2 = n_3 + n_4}} A_{n_1} A_{n_2} A_{n_3} A_{n_4} (2s_{I,n_1} s_{I,n_2} s_{I,n_3} s_{I,n_4} + s_{P,n_1} s_{P,n_2} s_{P,n_3} s_{P,n_4}) \\ &+ \frac{3}{2} k_4 \rho^2 R_{\text{ant}}^2 \sum_n A_n^4 s_{I,n}^2 s_{P,n}^2 \end{aligned} \quad (24)$$

and

$$\begin{aligned} t_{I,0}^{(k)} t_{P,0}^{(k)} &\approx t_{I,0}^{(k)} t_{P,0}^{(k-1)} + t_{I,0}^{(k-1)} t_{P,0}^{(k)} - t_{I,0}^{(k-1)} t_{P,0}^{(k-1)} \\ &= \text{Tr}(t_{P,0}^{(k-1)} \mathbf{C}_{I,0} \mathbf{V}^{(k)}) + \text{Tr}(t_{I,0}^{(k-1)} \mathbf{C}_{P,0} \mathbf{V}^{(k)}) - t_{I,0}^{(k-1)} t_{P,0}^{(k-1)} \end{aligned} \quad (38)$$

The second approximation holds since  $t_{I/P,0}$  are real. Therefore, we have

$$\begin{aligned} \tilde{z}(\mathbf{V}^{(k)}) &= \text{Tr}(\mathbf{A}^{(k)} \mathbf{V}^{(k)}) \\ &\quad - \frac{3k_4 \rho^2 R_{\text{ant}}^2}{8} \sum_{n=-N+1}^{N-1} 2t_{I,n}^{(k-1)} (t_{I,n}^{(k-1)})^* + t_{P,n}^{(k-1)} (t_{P,n}^{(k-1)})^* \\ &\quad - \frac{3k_4 \rho^2 R_{\text{ant}}^2}{2} t_{I,0}^{(k-1)} t_{P,0}^{(k-1)} \end{aligned} \quad (39)$$

where the Hermitian matrix  $\mathbf{A}^{(k)}$  is

$$\begin{aligned} \mathbf{A}^{(k)} &= \frac{k_2 \rho R_{\text{ant}}}{2} (\mathbf{C}_{I,0} + \mathbf{C}_{P,0}) \\ &\quad + \frac{3k_4 \rho^2 R_{\text{ant}}^2}{8} \sum_{n=-N+1}^{N-1} 2 \left( (t_{I,n}^{(k-1)})^* \mathbf{C}_{I,n} + t_{I,n}^{(k-1)} \mathbf{C}_{I,n}^H \right) \\ &\quad + \left( (t_{P,n}^{(k-1)})^* \mathbf{C}_{P,n} + t_{P,n}^{(k-1)} \mathbf{C}_{P,n}^H \right) \\ &\quad + \frac{3k_4 \rho^2 R_{\text{ant}}^2}{2} (t_{P,0}^{(k-1)} \mathbf{C}_{I,0} + t_{I,0}^{(k-1)} \mathbf{C}_{P,0}) \end{aligned} \quad (40)$$

Plug 39 into problem 33 and solve it by iterative interior-point method. Denote the optimal IRS matrix as  $\mathbf{V}^*$ . If  $\text{rank}(\mathbf{V}^*) = 1$ , the optimal phase shift vector  $\bar{\mathbf{v}}^*$  is attained by eigenvalue decomposition (EVD). Otherwise, a best feasible candidate  $\bar{\mathbf{v}}^*$  can be extracted through Gaussian randomization method [10]. First, we perform EVD on  $\mathbf{V}^*$  as  $\mathbf{V}^* = \mathbf{U}_{\mathbf{V}^*} \mathbf{\Sigma}_{\mathbf{V}^*} \mathbf{U}_{\mathbf{V}^*}^H$ . Then, we generate  $R$  random CSCG vectors  $\mathbf{r}_r \sim \mathcal{CN}(\mathbf{0}, \mathbf{I}_{L+1})$ ,  $r = 1, \dots, R$  and construct the corresponding candidates  $\bar{\mathbf{v}}_r = \mathbf{U}_{\mathbf{V}^*} \mathbf{\Sigma}_{\mathbf{V}^*}^{\frac{1}{2}} \mathbf{r}_r$ . Next, the optimal solution  $\bar{\mathbf{v}}^*$  is approximated by the one achieving maximum objective value of 33. Finally, we can retrieve the phase shift as  $\theta_l = \arg(v_l^*/v_{L+1}^*)$ . The algorithm for the phase optimization subproblem is summarized in Algorithm 1.

The waveform optimization subproblem is formed as follows. For a given  $\mathbf{V}$ , problem 32 reduces to

$$\begin{aligned} \max_{\mathbf{w}_I, \mathbf{w}_P, \rho} \quad & \sum_n \log_2 \left( 1 + \frac{(1-\rho)|w_{I,n}|^2 \text{Tr}(\mathbf{R}_n \mathbf{V})}{\sigma_n^2} \right) \\ \text{s.t.} \quad & \frac{1}{2} (\mathbf{w}_I^H \mathbf{w}_I + \mathbf{w}_P^H \mathbf{w}_P) \leq P, \\ & z(\mathbf{w}_I, \mathbf{w}_P, \rho) \geq \bar{z} \end{aligned} \quad (41)$$

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#### Algorithm 1 IRS Optimization

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- 1: **Input**  $\mathbf{w}_I, \mathbf{w}_P, \rho$
  - 2: **Initialize**  $k = 0, \mathbf{V}^{(0)}, t_{I/P,n}^{(0)} \forall n$
  - 3: **repeat**
  - 4:    $k = k + 1$
  - 5:   Update SDR matrix  $\mathbf{A}^{(k)}$  by 40
  - 6:   Obtain IRS matrix  $\mathbf{V}^{(k)}$  by solving problem 33
  - 7:   Update auxiliary  $t_{I/P,n}^{(k)} \forall n$  by 35 for SCA
  - 8: **until**  $R^{(k)} - R^{(k-1)} \leq \epsilon$
  - 9: Generate CSCG random vectors  $\mathbf{r}_r \sim \mathcal{CN}(\mathbf{0}, \mathbf{I}_{L+1}) \forall r$
  - 10: Perform EVD  $\mathbf{V}^* = \mathbf{U}_{\mathbf{V}^*} \mathbf{\Sigma}_{\mathbf{V}^*} \mathbf{U}_{\mathbf{V}^*}^H$
  - 11: Construct candidate IRS vectors  $\bar{\mathbf{v}}_r = \mathbf{U}_{\mathbf{V}^*} \mathbf{\Sigma}_{\mathbf{V}^*}^{\frac{1}{2}} \mathbf{r}_r \forall r$  and corresponding matrices  $\mathbf{V}_r = \bar{\mathbf{v}}_r \bar{\mathbf{v}}_r^H \forall r$
  - 12: Select the best solution  $\mathbf{V}_r^*$  for problem 33 and corresponding  $\mathbf{v}_r^*$
  - 13: Compute IRS phase shift by  $\theta_l = \arg(v_l^*/v_{L+1}^*) \forall l$
  - 14: **Output**  $\theta_l, l = 1, \dots, L$
- 

Similarly, define  $\mathbf{M} = \mathbf{h}^* \mathbf{h}^T$  and let  $\mathbf{M}_n$  keep the  $n$ -th ( $n = -N+1, \dots, N-1$ ) diagonal of  $\mathbf{M}$  and null the remaining entries. Since  $\mathbf{M} \succ 0$ , we have  $\mathbf{M}_{-n} = \mathbf{M}_n^H$ . Hence, 18 is transformed to 42. Introduce auxiliary variables

$$\begin{aligned} t'_{I/P,n} &= \mathbf{w}_{I/P}^H \mathbf{M}_n \mathbf{w}_{I/P} \\ &= \text{Tr}(\mathbf{M}_n \mathbf{w}_{I/P} \mathbf{w}_{I/P}^H) \\ &= \text{Tr}(\mathbf{M}_n \mathbf{W}_{I/P}) \end{aligned} \quad (43)$$

where  $\mathbf{W}_{I/P} = \mathbf{w}_{I/P} \mathbf{w}_{I/P}^H$ . Therefore, 42 rewrites as

$$\begin{aligned} z &= \frac{1}{2} k_2 \rho R_{\text{ant}} (t'_{I,0} + t'_{P,0}) \\ &\quad + \frac{3}{8} k_4 \rho^2 R_{\text{ant}}^2 \sum_{n=-N+1}^{N-1} 2t'_{I,n} t'_{I,n}^* + t'_{P,n} t'_{P,n}^* \\ &\quad + \frac{3}{2} k_4 \rho^2 R_{\text{ant}}^2 t'_{I,0} t'_{P,0} \end{aligned} \quad (44)$$

At iteration  $k$ , the second-order terms are approximated by first-order Taylor series as

$$\begin{aligned} t'_{I/P,n}^{(k)} (t'_{I/P,n}^{(k)})^* &\approx 2\Re \left\{ t'_{I/P,n}^{(k)} (t'_{I/P,n}^{(k-1)})^* \right\} - t'_{I/P,n}^{(k-1)} (t'_{I/P,n}^{(k-1)})^* \\ &= 2\Re \left\{ \text{Tr}((t'_{I/P,n}^{(k-1)})^* \mathbf{M}_n \mathbf{W}_{I/P}^{(k)}) \right\} - t'_{I/P,n}^{(k-1)} (t'_{I/P,n}^{(k-1)})^* \\ &= \text{Tr} \left( (t'_{I/P,n}^{(k-1)})^* \mathbf{M}_n \mathbf{W}_{I/P}^{(k)} \right) + \text{Tr} (t'_{I/P,n}^{(k-1)} \mathbf{M}_n^H \mathbf{W}_{I/P}^{(k)}) \\ &\quad - t'_{I/P,n}^{(k-1)} (t'_{I/P,n}^{(k-1)})^* \end{aligned} \quad (45)$$

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$$\begin{aligned} z &= \frac{1}{2} k_2 \rho R_{\text{ant}} (\mathbf{h}^H \mathbf{M}_{I,0} \mathbf{h} + \mathbf{h}^H \mathbf{M}_{P,0} \mathbf{h}) \\ &\quad + \frac{3}{8} k_4 \rho^2 R_{\text{ant}}^2 \sum_{n=-N+1}^{N-1} 2(\mathbf{h}^H \mathbf{M}_{I,n} \mathbf{h})(\mathbf{h}^H \mathbf{M}_{I,n} \mathbf{h})^* + (\mathbf{h}^H \mathbf{M}_{P,n} \mathbf{h})(\mathbf{h}^H \mathbf{M}_{P,n} \mathbf{h})^* \\ &\quad + \frac{3}{2} k_4 \rho^2 R_{\text{ant}}^2 (\mathbf{h}^H \mathbf{M}_{I,0} \mathbf{h})(\mathbf{h}^H \mathbf{M}_{P,0} \mathbf{h}) \end{aligned} \quad (34)$$

and

$$\begin{aligned} t'_{I,0}{}^{(k)} t'_{P,0}{}^{(k)} &\approx t'_{I,0}{}^{(k)} t'_{P,0}{}^{(k-1)} + t'_{I,0}{}^{(k-1)} t'_{P,0}{}^{(k)} - t'_{I,0}{}^{(k-1)} t'_{P,0}{}^{(k-1)} \\ &= \text{Tr} \left( t'_{P,0}{}^{(k-1)} \mathbf{M}_0 \mathbf{W}_{I,0}^{(k)} \right) + \text{Tr} \left( t'_{I,0}{}^{(k-1)} \mathbf{M}_0 \mathbf{W}_{P,0}^{(k)} \right) - t'_{I,0}{}^{(k-1)} t'_{P,0}{}^{(k-1)} \end{aligned} \quad (46)$$

Therefore, we have

$$\begin{aligned} \tilde{z}(\mathbf{W}_I^{(k)}, \mathbf{W}_P^{(k)}, \rho^{(k-1)}) &= \text{Tr}(\mathbf{A}_I^{(k)} \mathbf{W}_I^{(k)}) + \text{Tr}(\mathbf{A}_P^{(k)} \mathbf{W}_P^{(k)}) \\ &\quad - \frac{3k_4(\rho^{(k-1)})^2 R_{\text{ant}}^2}{8} \sum_{n=-N+1}^{N-1} 2 t'_{I,n}{}^{(k-1)} (t'_{I,n}{}^{(k-1)})^* \\ &\quad - \frac{3k_4(\rho^{(k-1)})^2 R_{\text{ant}}^2}{2} t'_{I,0}{}^{(k-1)} t'_{P,0}{}^{(k-1)} \end{aligned} \quad (47)$$

where the Hermitian matrices  $\mathbf{A}_I^{(k)}$  and  $\mathbf{A}_P^{(k)}$  are

$$\begin{aligned} \mathbf{A}_I^{(k)} &= \frac{k_2 \rho^{(k-1)} R_{\text{ant}}}{2} \mathbf{M}_0 \\ &\quad + \frac{3k_4(\rho^{(k-1)})^2 R_{\text{ant}}^2}{8} \sum_{n=-N+1}^{N-1} 2 \left( (t'_{I,n}{}^{(k-1)})^* \mathbf{M}_n + t'_{I,n}{}^{(k-1)} \mathbf{M}_n^H \right) \\ &\quad + \frac{3k_4(\rho^{(k-1)})^2 R_{\text{ant}}^2}{2} t'_{P,0}{}^{(k-1)} \mathbf{M}_0 \end{aligned} \quad (48)$$

$$\begin{aligned} \mathbf{A}_P^{(k)} &= \frac{k_2 \rho^{(k-1)} R_{\text{ant}}}{2} \mathbf{M}_0 \\ &\quad + \frac{3k_4(\rho^{(k-1)})^2 R_{\text{ant}}^2}{8} \sum_{n=-N+1}^{N-1} (t'_{P,n}{}^{(k-1)})^* \mathbf{M}_n + t'_{P,n}{}^{(k-1)} \mathbf{M}_n^H \\ &\quad + \frac{3k_4(\rho^{(k-1)})^2 R_{\text{ant}}^2}{2} t'_{I,0}{}^{(k-1)} \mathbf{M}_0 \end{aligned} \quad (49)$$

Plug 47 into problem 41 and solve it by iterative interior-point method. Given the optimal waveform matrices  $\mathbf{W}_I$  and  $\mathbf{W}_P$ , the best rank-1 solution  $\mathbf{w}_I$  and  $\mathbf{w}_P$  can be obtained through randomization method. Details are omitted here. The algorithm for the waveform optimization subproblem is summarized in Algorithm 2.

## Algorithm 2 Waveform Optimization

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1: Input  $\mathbf{V}$ 
2: Initialize  $k = 0$ ,  $\mathbf{w}_{I/P}^{(0)}$ ,  $\rho^{(0)}$ ,  $t'_{I/P,n}{}^{(0)} \forall n$ 
3: repeat
4:    $k = k + 1$ 
5:   Update SDR matrices  $\mathbf{A}_{I/P}^{(k)}$  by 48 and 49
6:   Obtain waveform matrices  $\mathbf{W}_{I/P}^{(k)}$  and  $\rho^{(k)}$  by solving
     problem 41
7:   Update auxiliary  $t'_{I/P,n}{}^{(k)}$   $\forall n$  by 43 for SCA
8:   until  $t'_{I,n}{}^{(k)} - t'_{I,n}{}^{(k-1)} \leq \epsilon$ 
9:   Generate CSCG random vectors  $\mathbf{r}_r \sim \mathcal{CN}(\mathbf{0}, \mathbf{I}_N) \forall r$ 
10:  Perform EVD  $\mathbf{W}_{I/P}^* = \mathbf{U} \mathbf{w}_{I/P}^* \Sigma \mathbf{w}_{I/P}^* \mathbf{U}^H$ 
11:  Construct candidate waveform vectors  $\mathbf{w}_{I/P,r} = \mathbf{U} \mathbf{w}_{I/P}^* \Sigma^{\frac{1}{2}} \mathbf{w}_{I/P}^* \mathbf{r}_r \forall r$  and corresponding matrices
      $\mathbf{W}_{I/P,r} = \mathbf{w}_{I/P,r} \mathbf{w}_{I/P,r}^H \forall r$ 
12:  Select the best solution pair  $\mathbf{W}_{I,r}^*$ ,  $\mathbf{W}_{P,r}^*$  for problem 41
     and corresponding  $\mathbf{w}_{I,r}^*$ ,  $\mathbf{w}_{P,r}^*$ 
13: Output  $\mathbf{w}_I^*$ ,  $\mathbf{w}_P^*$ ,  $\rho^*$ 

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$$\begin{aligned} z &= \frac{1}{2} k_2 \rho R_{\text{ant}} (\mathbf{w}_I^H \mathbf{M}_0 \mathbf{w}_I + \mathbf{w}_P^H \mathbf{M}_0 \mathbf{w}_P) \\ &\quad + \frac{3}{8} k_4 \rho^2 R_{\text{ant}}^2 \sum_{n=-N+1}^{N-1} 2 (\mathbf{w}_I^H \mathbf{M}_n \mathbf{w}_I) (\mathbf{w}_I^H \mathbf{M}_n \mathbf{w}_I)^* + (\mathbf{w}_P^H \mathbf{M}_n \mathbf{w}_P) (\mathbf{w}_P^H \mathbf{M}_n \mathbf{w}_P)^* \\ &\quad + \frac{3}{2} k_4 \rho^2 R_{\text{ant}}^2 (\mathbf{w}_I^H \mathbf{M}_0 \mathbf{w}_I) (\mathbf{w}_P^H \mathbf{M}_0 \mathbf{w}_P) \end{aligned} \quad (42)$$