

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. 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 α 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 α 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 ρ such that the PS ratio is coupled with waveform design. Perfect synchronization is assumed among the three parties in both scenarios.

A. Transmit Signal

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 ($n = 1, \dots, N$).

1) *Modulated Information Waveform*: Let $\tilde{x}_{I,k,n}$ be the information symbol of user 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 f_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 baseband equivalent channels from the AP to users, from the AP to the IRS, and from the IRS to users as $\mathbf{H}_D \in \mathbb{C}^{K \times N}$, $\mathbf{H}_I' \in \mathbb{C}^{L \times N}$, and $\mathbf{H}_R^H \in \mathbb{C}^{K \times NL}$ respectively. At subband n , the frequency response of direct and reflective links write as $\mathbf{h}_{D,n} = [h_{D,1,n}, \dots, h_{D,K,n}]^H \in \mathbb{C}^{K \times 1}$ and $\mathbf{H}_{R,n}^H = [\mathbf{h}_{R,1,n}, \dots, \mathbf{h}_{R,K,n}]^H \in \mathbb{C}^{K \times L}$ with $\mathbf{h}_{R,k,n} = [h_{R,k,n,1}, \dots, h_{R,k,n,L}] \in \mathbb{C}^{1 \times L}$. Similarly, the n -th incident channel is given by $\mathbf{h}_{I,n} = [h_{I,n,1}, \dots, h_{I,n,L}]^H \in \mathbb{C}^{L \times 1}$. To decouple the impact of IRS operation on the incident link, we construct a block-diagonal matrix $\mathbf{H}_I \triangleq \text{diag}\{\mathbf{h}_{I,1}, \dots, \mathbf{h}_{I,N}\} \in \mathbb{C}^{NL \times N}$. Element l of the IRS receives a superposed waveform through the multipath channel, then redistributes it by adjusting the amplitude reflection coefficient $\beta_l \in [0, 1]$ and phase shift $\theta_l \in [0, 2\pi)$. Each passive reflector absorbs a small portion $(1 - \beta_l)$ of the signal to support CSI decoding and impedance matching. On top of this, the IRS matrix per subband is constructed by collecting the reflection coefficients onto its diagonal entries as $\mathbf{\Theta}_0 = \text{diag}\{\beta_1 e^{j\theta_1}, \dots, \beta_L e^{j\theta_L}\} \in \mathbb{C}^{L \times L}$. Finally, the IRS matrix is formed by $\mathbf{\Theta} = \text{diag}\{\underbrace{\mathbf{\Theta}_0, \dots, \mathbf{\Theta}_0}_{N \text{ times}}\} \in \mathbb{C}^{NL \times NL}$.

The IRS-aided extra link can be modeled as a concatenation of the AP-IRS channel, the IRS reflection matrix, and the IRS-user channel. Both direct and IRS-aided link contributes to the composite channel $\mathbf{H} \in \mathbb{C}^{K \times N}$ as

$$\mathbf{H} = \mathbf{H}_D + \mathbf{H}_R^H \mathbf{\Theta} \mathbf{H}_I \quad (4)$$

whose (k, n) -th entry

$$h_{k,n} = h_{D,k,n} + \mathbf{h}_{R,k,n}^H \mathbf{\Theta}_0 \mathbf{h}_{I,n} \quad (5)$$

represents the overall channel gain of user k at subband n . On top of this, the n -th subchannel for all users $\mathbf{h}_n \in \mathbb{C}^{K \times 1}$ can be expressed as

$$\mathbf{h}_n = \mathbf{h}_{D,n} + \mathbf{H}_{R,n}^H \mathbf{\Theta}_0 \mathbf{h}_{I,n} \quad (6)$$

Define $\mathbf{v} = [e^{j\theta_1}, \dots, e^{j\theta_L}]^H \in \mathbb{C}^{L \times 1}$ and $\Phi_n^H = \mathbf{H}_{R,n}^H \text{diag}\{\mathbf{h}_{I,n}\} \in \mathbb{C}^{K \times L}$. Therefore, 6 rewrites as

$$\mathbf{h}_n = \mathbf{h}_{D,n} + \Phi_n^H \mathbf{v} \quad (7)$$

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

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

D. Information Decoder

One major benefit of using proposed waveform is that the deterministic power term $y_{P,k}(t)$ bears no information and creates no interference to the modulated information term $y_{I,k}(t)$. Hence, each user treats the information signals from other users as interference such that the SINR at subband n of user k is

$$\gamma_{k,n} = \frac{(1-\rho)(h_{k,n}w_{I,k,n})(h_{k,n}w_{I,k,n})^*}{\sum_{j=1, j \neq k}^K (1-\rho)(h_{k,n}w_{I,j,n})(h_{k,n}w_{I,j,n})^* + \sigma_n^2} \quad (9)$$

where σ_n^2 is the sum variance of the Gaussian noise at the RF-band and those introduced during the RF-to-BB conversion on subband n . Therefore, the achievable rate of user k is expressed as

$$R_k(\mathbf{W}_I, \mathbf{\Theta}_0, \rho) = \sum_{n=1}^N \log_2(1 + \gamma_{k,n}) \quad (10)$$

A significant conclusion in [6] indicates that the rate 10 is always achievable with or without waveform cancellation, through either subtracting the deterministic power component or constructing a translated codebook.

E. Energy Harvester

Note that the information and power component $y_{I,k}(t)$ and $y_{P,k}(t)$ have different influence on the output DC current. Consider a nonlinear diode model based on the Taylor expansion of a small signal model [6], [5], which highlights the dependency of the harvester output DC current on the received waveform as

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

where R_{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. Once the composite channel response $h_{k,n}$ is fixed, the corresponding information and power weight $w_{I,k,n}$, $w_{P,k,n}$ are thus optimized such that the randomness comes from the input distribution $\tilde{x}_{k,n}$. Therefore, we first

extract the DC component based on $h_{k,n}$, $w_{I,k,n}$, $w_{P,k,n}$ by $\mathcal{A}\{\cdot\}$ and then take the expectation over $\tilde{x}_{k,n}$ by $\mathcal{E}\{\cdot\}$. With the assumption of evenly spaced frequencies, $\mathcal{E}\{y^i(t)\} = 0$ for odd i and the related terms has zero contribution to DC components. [5] also demonstrated that to maximize i_k , it suffices to maximize the monotonic target function truncated to the n_0 order

$$z_k(\mathbf{W}_I, \mathbf{W}_P, \mathbf{\Theta}_0, \rho) = \sum_{i \text{ even}, i \geq 2}^{n_0} k_i \rho^{i/2} R_{\text{ant}}^{i/2} \mathcal{E} \{ \mathcal{A} \{ y_k(t)^i \} \} \quad (12)$$

where $k_i = i_s / i!(nv_t)^i$. We take $n_0 = 4$ to investigate the fundamental impact of diode nonlinearity on power transfer. Note that $\mathcal{E}\{\mathcal{A}\{y_{I,k}(t)y_{P,k}(t)\}\} = \mathcal{E}\{\mathcal{A}\{y_{I,k}^3(t)y_{P,k}(t)\}\} = \mathcal{E}\{\mathcal{A}\{y_{I,k}(t)y_{P,k}^3(t)\}\} = 0$, $\mathcal{E}\{\mathcal{A}\{y_{I,k}^2(t)y_{P,k}^2(t)\}\} = \mathcal{A}\{\mathcal{E}\{y_{I,k}^2(t)\}\}\mathcal{A}\{y_{P,k}^2(t)\}$, and the remaining terms are expressed by 13 – 20. It is noteworthy that modulation provides a power gain to the nonlinear terms in the output DC current as $\mathcal{E}\{|\tilde{x}_{k,n}|^2\} = 1$ and $\mathcal{E}\{|\tilde{x}_{k,n}|^4\} = 2$. Therefore, 12 reduces to 21.

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

$$C_{R-I}(P) \triangleq \left\{ (R, I) : R \leq \sum_{k=1}^K u_{I,k} R_k, I \leq \sum_{k=1}^K u_{P,k} z_k, \frac{1}{2}(\mathbf{w}_I^H \mathbf{w}_I + \mathbf{w}_P^H \mathbf{w}_P) \leq P \right\} \quad (22)$$

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 $h_n = A_n e^{j\tilde{\psi}_n}$, $w_{I,n} = s_{I,n} e^{j\phi_n}$, $w_{P,n} = s_{P,n} e^{j\phi_n}$. The WSR-E region can be obtained through a rate maximization problem subject to transmit power and output DC current constraints

$$\begin{aligned} \max_{\mathbf{w}_I, \mathbf{w}_P, \mathbf{v}, \rho} \quad & \sum_n \log_2 \left(1 + \frac{(1-\rho)|(h_{D,n} + \Phi_n^H \mathbf{v})w_{I,n}|^2}{\sigma_n^2} \right) \\ \text{s.t.} \quad & \frac{1}{2}(\mathbf{w}_I^H \mathbf{w}_I + \mathbf{w}_P^H \mathbf{w}_P) \leq P, \\ & z(\mathbf{w}_I, \mathbf{w}_P, \mathbf{v}, \rho) \geq \bar{z}, \\ & |v_l| = 1, \quad l = 1, \dots, L \end{aligned} \quad (23)$$

Problem 23 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 23. 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

$$\theta_{n,l}^* = \angle h_{D,n} - \angle h_{R,n,l} - \angle h_{I,n,l} \quad (24)$$

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 9, 10 and 21 that the optimal phase of information and power waveforms are matched to composite frequency response as

$$\phi_{I,n}^* = \phi_{P,n}^* = -\bar{\psi}_n \quad (25)$$

With all the phases determined, the original problem 23 is reduced to

$$\begin{aligned} \max_{\mathbf{s}_I, \mathbf{s}_P, \rho} \quad & \sum_n \log_2 \left(1 + \frac{(1-\rho)A_n^2 s_{I,n}^2}{\sigma_n^2} \right) \\ \text{s.t.} \quad & \frac{1}{2}(\mathbf{s}_I^H \mathbf{s}_I + \mathbf{s}_P^H \mathbf{s}_P) \leq P, \\ & z(\mathbf{s}_I, \mathbf{s}_P, \rho) \geq \bar{z} \end{aligned} \quad (26)$$

with z given by 27. It can be transformed to an equivalent problem by introducing an auxiliary variable t_0

$$\begin{aligned} \min_{\mathbf{s}_I, \mathbf{s}_P, \rho} \quad & \frac{1}{t_0} \\ \text{s.t.} \quad & \frac{1}{2}(\mathbf{s}_I^H \mathbf{s}_I + \mathbf{s}_P^H \mathbf{s}_P) \leq P, \\ & \frac{t_0}{\prod_n \left(1 + \frac{(1-\rho)A_n^2 s_{I,n}^2}{\sigma_n^2} \right)} \leq 1, \\ & \frac{\bar{z}}{z(\mathbf{s}_I, \mathbf{s}_P, \rho)} \leq 1 \end{aligned} \quad (28)$$

28 is a Reversed Geometric Program which can be transformed to standard Geometric Program (GP). The basic idea is to

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

$$= \frac{1}{2} \sum_n h_{k,n} h_{k,n}^* \mathbf{w}_{I,n}^H \mathbf{J}_K \mathbf{w}_{I,n} \quad (14)$$

$$\mathcal{E} \{ \mathcal{A} \{ y_{I,k}^4(t) \} \} = \frac{3}{4} \sum_{j_1, j_2, j_3, j_4} \sum_{\substack{n_1, n_2, n_3, n_4 \\ n_1 + n_2 = n_3 + n_4}} (h_{k,n_1} w_{I,j_1,n_1}) (h_{k,n_2} w_{I,j_2,n_2}) (h_{k,n_3} w_{I,j_3,n_3})^* (h_{k,n_4} w_{I,j_4,n_4})^* \quad (15)$$

$$= \frac{3}{4} \sum_{\substack{n_1, n_2, n_3, n_4 \\ n_1 + n_2 = n_3 + n_4}} h_{k,n_3}^* h_{k,n_1} h_{k,n_4}^* h_{k,n_2} (\mathbf{w}_{I,n_3}^H \mathbf{J}_K \mathbf{w}_{I,n_1}) (\mathbf{w}_{I,n_4}^H \mathbf{J}_K \mathbf{w}_{I,n_2}) \quad (16)$$

$$\mathcal{A} \{ y_{P,k}^2(t) \} = \frac{1}{2} \sum_{j_1, j_2} \sum_n (h_{k,n} w_{P,j_1,n}) (h_{k,n} w_{P,j_2,n})^* \quad (17)$$

$$= \frac{1}{2} \sum_n h_{k,n} h_{k,n}^* \mathbf{w}_{P,n}^H \mathbf{J}_K \mathbf{w}_{P,n} \quad (18)$$

$$\mathcal{A} \{ y_{P,k}^4(t) \} = \frac{3}{8} \sum_{j_1, j_2, j_3, j_4} \sum_{\substack{n_1, n_2, n_3, n_4 \\ n_1 + n_2 = n_3 + n_4}} (h_{k,n_1} w_{P,j_1,n_1}) (h_{k,n_2} w_{P,j_2,n_2}) (h_{k,n_3} w_{P,j_3,n_3})^* (h_{k,n_4} w_{P,j_4,n_4})^* \quad (19)$$

$$= \frac{3}{8} \sum_{\substack{n_1, n_2, n_3, n_4 \\ n_1 + n_2 = n_3 + n_4}} h_{k,n_3}^* h_{k,n_1} h_{k,n_4}^* h_{k,n_2} (\mathbf{w}_{P,n_3}^H \mathbf{J}_K \mathbf{w}_{P,n_1}) (\mathbf{w}_{P,n_4}^H \mathbf{J}_K \mathbf{w}_{P,n_2}) \quad (20)$$

$$\begin{aligned} z_k &= k_2 \rho R_{\text{ant}} (\mathcal{E} \{ \mathcal{A} \{ y_{I,k}^2(t) \} \} + \mathcal{A} \{ y_{P,k}^2(t) \}) + k_4 \rho^2 R_{\text{ant}}^2 (\mathcal{E} \{ \mathcal{A} \{ y_{I,k}^4(t) \} \} + \mathcal{A} \{ y_{P,k}^4(t) \}) + 6 \mathcal{E} \{ \mathcal{A} \{ y_{I,k}^2(t) \} \} \mathcal{A} \{ y_{P,k}^2(t) \}) \\ &= \frac{1}{2} k_2 \rho R_{\text{ant}} \sum_n h_{k,n} h_{k,n}^* (\mathbf{w}_{I,n}^H \mathbf{J}_K \mathbf{w}_{I,n} + \mathbf{w}_{P,n}^H \mathbf{J}_K \mathbf{w}_{P,n}) \\ &\quad + \frac{3}{8} k_4 \rho^2 R_{\text{ant}}^2 \sum_{\substack{n_1, n_2, n_3, n_4 \\ n_1 + n_2 = n_3 + n_4}} h_{k,n_3}^* h_{k,n_1} h_{k,n_4}^* h_{k,n_2} (2(\mathbf{w}_{I,n_3}^H \mathbf{J}_K \mathbf{w}_{I,n_1}) (\mathbf{w}_{I,n_4}^H \mathbf{J}_K \mathbf{w}_{I,n_2}) + (\mathbf{w}_{P,n_3}^H \mathbf{J}_K \mathbf{w}_{P,n_1}) (\mathbf{w}_{P,n_4}^H \mathbf{J}_K \mathbf{w}_{P,n_2})) \\ &\quad + \frac{3}{2} k_4 \rho^2 R_{\text{ant}}^2 \sum_n h_{k,n}^2 h_{k,n}^2 (\mathbf{w}_{I,n}^H \mathbf{J}_K \mathbf{w}_{I,n}) (\mathbf{w}_{P,n}^H \mathbf{J}_K \mathbf{w}_{P,n}) \end{aligned} \quad (21)$$

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 28 is equivalent to

$$\begin{aligned} \min_{\mathbf{s}_I, \mathbf{s}_P, \rho} \quad & \frac{1}{t_0} \\ \text{s.t.} \quad & \frac{1}{2}(\mathbf{s}_I^H \mathbf{s}_I + \mathbf{s}_P^H \mathbf{s}_P) \leq P, \\ & t_0 \prod_n \left(\frac{1}{\gamma_{I,n,1}} \right)^{-\gamma_{I,n,1}} \left(\frac{\bar{\rho} A_n^2 s_{I,n}^2}{\sigma_n^2 \gamma_{I,n,2}} \right)^{-\gamma_{I,n,2}} \leq 1, \\ & \bar{z} \prod_{m_P} \left(\frac{g_{P,m_P}(\mathbf{s}_I, \mathbf{s}_P, \rho)}{\gamma_{P,m_P}} \right)^{-\gamma_{P,m_P}} \leq 1, \\ & \rho + \bar{\rho} \leq 1 \end{aligned} \quad (29)$$

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 $\sum_{m_P=1}^{M_P} \gamma_{m_P} = 1$. 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 choose

$$\gamma_{I,n,1}^{(i)} = \frac{1}{1 + \frac{\bar{\rho}^{(i-1)} A_n^2 s_{I,n}^{(i-1)2}}{\sigma_n^2}}, \quad n = 1, \dots, N, \quad (30)$$

$$\gamma_{I,n,2}^{(i)} = \frac{\frac{\bar{\rho}^{(i-1)} A_n^2 s_{I,n}^{(i-1)2}}{\sigma_n^2}}{1 + \frac{\bar{\rho}^{(i-1)} A_n^2 s_{I,n}^{(i-1)2}}{\sigma_n^2}}, \quad n = 1, \dots, N, \quad (31)$$

$$\gamma_{P,m_P}^{(i)} = \frac{g_{P,m_P}(\mathbf{s}_I^{(i-1)}, \mathbf{s}_P^{(i-1)}, \rho^{(i-1)})}{z(\mathbf{s}_I^{(i-1)}, \mathbf{s}_P^{(i-1)}, \rho^{(i-1)})}, \quad m_P = 1, \dots, M_P \quad (32)$$

and then solve problem 29.

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

$$\begin{aligned} |h_{D,n} + \Phi_n^H \mathbf{v}|^2 &= |h_{D,n}|^2 + h_{D,n}^* \Phi_n^H \mathbf{v} + \mathbf{v}^H \Phi_n h_{D,n} + \mathbf{v}^H \Phi_n \Phi_n^H \mathbf{v} \\ &= \bar{\mathbf{v}}^H \mathbf{R} \bar{\mathbf{v}} = \text{Tr}(\mathbf{R}_n \bar{\mathbf{v}} \bar{\mathbf{v}}^H) = \text{Tr}(\mathbf{R}_n \mathbf{V}) \end{aligned} \quad (33)$$

where t is an auxiliary variable with unit modulus and

$$\mathbf{R}_n = \begin{bmatrix} \Phi_n \Phi_n^H & \Phi_n h_{D,n} \\ h_{D,n}^* \Phi_n^H & h_{D,n}^* h_{D,n} \end{bmatrix}, \quad \bar{\mathbf{v}} = \begin{bmatrix} \mathbf{v} \\ t \end{bmatrix}, \quad \bar{\mathbf{V}} = \bar{\mathbf{v}} \bar{\mathbf{v}}^H \quad (34)$$

Hence, 23 is transformed to

$$\begin{aligned} \max_{\mathbf{w}_I, \mathbf{w}_P, \mathbf{V}, \rho} \quad & \sum_n \log_2 \left(1 + \frac{(1-\rho)|w_{I,n}|^2 \text{Tr}(\mathbf{R}_n \mathbf{V})}{\sigma_n^2} \right) \\ \text{s.t.} \quad & \frac{1}{2}(\mathbf{w}_I^H \mathbf{w}_I + \mathbf{w}_P^H \mathbf{w}_P) \leq P, \\ & z(\mathbf{w}_I, \mathbf{w}_P, \mathbf{V}, \rho) \geq \bar{z}, \\ & \mathbf{V}_{l,l} = 1, l = 1, \dots, L+1, \\ & \mathbf{V} \succeq 0, \\ & \text{rank}(\mathbf{V}) = 1 \end{aligned} \quad (35)$$

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 35 reduces to

$$\begin{aligned} \max_{\mathbf{V}} \quad & \sum_n \log_2 \left(1 + \frac{(1-\rho)|w_{I,n}|^2 \text{Tr}(\mathbf{R}_n \mathbf{V})}{\sigma_n^2} \right) \\ \text{s.t.} \quad & z(\mathbf{V}) \geq \bar{z}, \\ & \mathbf{V}_{l,l} = 1, l = 1, \dots, L+1, \\ & \mathbf{V} \succeq 0, \\ & \text{rank}(\mathbf{V}) = 1 \end{aligned} \quad (36)$$

To tackle the non-convex current constraint, we collect the channel matrices into $\Phi^H = [\Phi_1^H, \dots, \Phi_N^H] \in \mathbb{C}^{N \times L}$ 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 21 is transformed to 37. We further simplify it by introducing auxiliary variables

$$\begin{aligned} t_{I/P,n} &= \mathbf{h}^H \mathbf{M}_{I/P,n} \mathbf{h} \\ &= \text{Tr}(\mathbf{h} \mathbf{h}^H \mathbf{M}_{I/P,n}) \\ &= \text{Tr}(\mathbf{R}^H \mathbf{V} \mathbf{R} \mathbf{M}_{I/P,n}) \\ &= \text{Tr}(\mathbf{R} \mathbf{M}_{I/P,n} \mathbf{R}^H \mathbf{V}) \\ &= \text{Tr}(\mathbf{C}_{I/P,n} \mathbf{V}) \end{aligned} \quad (38)$$

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, 37 rewrites as

$$\begin{aligned} z &= \frac{1}{2} k_2 \rho R_{\text{ant}} (t_{I,0} + t_{P,0}) \\ &+ \frac{3}{8} k_4 \rho^2 R_{\text{ant}}^2 \sum_{n=-N+1}^{N-1} 2t_{I,n} t_{I,n}^* + t_{P,n} t_{P,n}^* \\ &+ \frac{3}{2} k_4 \rho^2 R_{\text{ant}}^2 t_{I,0} t_{P,0} \end{aligned} \quad (39)$$

$$\begin{aligned} z &= \frac{1}{2} k_2 \rho R_{\text{ant}} \sum_n A_n^2 (s_{I,n}^2 + s_{P,n}^2) + \frac{3}{8} k_4 \rho^2 R_{\text{ant}}^2 \sum_{\substack{n_1, n_2, n_3, n_4 \\ n_1 + n_2 = n_3 + n_4}} A_{n_1} A_{n_2} A_{n_3} A_{n_4} (2s_{I,n_1} s_{I,n_2} s_{I,n_3} s_{I,n_4} + s_{P,n_1} s_{P,n_2} s_{P,n_3} s_{P,n_4}) \\ &+ \frac{3}{2} k_4 \rho^2 R_{\text{ant}}^2 \sum_n A_n^4 s_{I,n}^2 s_{P,n}^2 \end{aligned} \quad (27)$$

We use first-order Taylor expansion to approximate the second-order terms in 39. Based on the variables optimized at iteration $k-1$, the local approximations at iteration k are [9]

$$\begin{aligned} t_{I/P,n}^{(k)} (t_{I/P,n}^{(k)})^* &\approx 2\Re \left\{ t_{I/P,n}^{(k)} (t_{I/P,n}^{(k-1)})^* \right\} - t_{I/P,n}^{(k-1)} (t_{I/P,n}^{(k-1)})^* \\ &= 2\Re \left\{ \text{Tr} \left((t_{I/P,n}^{(k-1)})^* \mathbf{C}_{I/P,n} \mathbf{V}^{(k)} \right) \right\} - t_{I/P,n}^{(k-1)} (t_{I/P,n}^{(k-1)})^* \\ &= \text{Tr} \left((t_{I/P,n}^{(k-1)})^* \mathbf{C}_{I/P,n} \mathbf{V}^{(k)} \right) + \text{Tr} (t_{I/P,n}^{(k-1)} \mathbf{C}_{I/P,n}^H \mathbf{V}^{(k)}) \\ &\quad - t_{I/P,n}^{(k-1)} (t_{I/P,n}^{(k-1)})^* \end{aligned} \quad (40)$$

and

$$\begin{aligned} t_{I,0}^{(k)} t_{P,0}^{(k)} &\approx t_{I,0}^{(k)} t_{P,0}^{(k-1)} + t_{I,0}^{(k-1)} t_{P,0}^{(k)} - t_{I,0}^{(k-1)} t_{P,0}^{(k-1)} \\ &= \text{Tr} (t_{P,0}^{(k-1)} \mathbf{C}_{I,0} \mathbf{V}^{(k)}) + \text{Tr} (t_{I,0}^{(k-1)} \mathbf{C}_{P,0} \mathbf{V}^{(k)}) - t_{I,0}^{(k-1)} t_{P,0}^{(k-1)} \end{aligned} \quad (41)$$

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

$$\begin{aligned} \tilde{z}(\mathbf{V}^{(k)}) &= \text{Tr}(\mathbf{A}^{(k)} \mathbf{V}^{(k)}) \\ &\quad - \frac{3k_4 \rho^2 R_{\text{ant}}^2}{8} \sum_{n=-N+1}^{N-1} 2t_{I,n}^{(k-1)} (t_{I,n}^{(k-1)})^* + t_{P,n}^{(k-1)} (t_{P,n}^{(k-1)})^* \\ &\quad - \frac{3k_4 \rho^2 R_{\text{ant}}^2}{2} t_{I,0}^{(k-1)} t_{P,0}^{(k-1)} \end{aligned} \quad (42)$$

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

$$\begin{aligned} \mathbf{A}^{(k)} &= \frac{k_2 \rho R_{\text{ant}}}{2} (\mathbf{C}_{I,0} + \mathbf{C}_{P,0}) \\ &\quad + \frac{3k_4 \rho^2 R_{\text{ant}}^2}{8} \sum_{n=-N+1}^{N-1} 2 \left((t_{I,n}^{(k-1)})^* \mathbf{C}_{I,n} + t_{I,n}^{(k-1)} \mathbf{C}_{I,n}^H \right) \\ &\quad + \left((t_{P,n}^{(k-1)})^* \mathbf{C}_{P,n} + t_{P,n}^{(k-1)} \mathbf{C}_{P,n}^H \right) \\ &\quad + \frac{3k_4 \rho^2 R_{\text{ant}}^2}{2} (t_{P,0}^{(k-1)} \mathbf{C}_{I,0} + t_{I,0}^{(k-1)} \mathbf{C}_{P,0}) \end{aligned} \quad (43)$$

Plug 42 into problem 36 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 $\mathbf{V}^* = \mathbf{U}_{\mathbf{V}^*} \boldsymbol{\Sigma}_{\mathbf{V}^*} \mathbf{U}_{\mathbf{V}^*}^H$. 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 $\bar{\mathbf{v}}_r = \mathbf{U}_{\mathbf{V}^*} \boldsymbol{\Sigma}_{\mathbf{V}^*}^{\frac{1}{2}} \mathbf{r}_r$. Next, the

optimal solution $\bar{\mathbf{v}}^*$ is approximated by the one achieving maximum objective value of 36. 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.

Algorithm 1 IRS Optimization

Input $\mathbf{w}_I, \mathbf{w}_P, \rho$
Initialize $k = 0, \mathbf{V}^{(0)}, t_{I/P,n}^{(0)} \forall n$
repeat
 4: $k = k + 1$
 5: Update SDR matrix $\mathbf{A}^{(k)}$ by 43
 6: Obtain IRS matrix $\mathbf{V}^{(k)}$ by solving problem 36
 7: Update auxiliary $t_{I/P,n}^{(k)} \forall n$ by 38 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 $\mathbf{V}^* = \mathbf{U}_{\mathbf{V}^*} \boldsymbol{\Sigma}_{\mathbf{V}^*} \mathbf{U}_{\mathbf{V}^*}^H$
 11: Construct candidate IRS vectors $\bar{\mathbf{v}}_r = \mathbf{U}_{\mathbf{V}^*} \boldsymbol{\Sigma}_{\mathbf{V}^*}^{\frac{1}{2}} \mathbf{r}_r \forall r$ 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 36 and corresponding \mathbf{v}_r^*
 13: Compute IRS phase shift by $\theta_l = \arg(v_l^*/v_{L+1}^*) \forall l$
 14: **Output** $\theta_l, l = 1, \dots, L$

The waveform optimization subproblem is formed as follows. For a given \mathbf{V} , problem 35 reduces to

$$\begin{aligned} \max_{\mathbf{w}_I, \mathbf{w}_P, \rho} \quad & \sum_n \log_2 \left(1 + \frac{(1-\rho)|w_{I,n}|^2 \text{Tr}(\mathbf{R}_n \mathbf{V})}{\sigma_n^2} \right) \\ \text{s.t.} \quad & \frac{1}{2} (\mathbf{w}_I^H \mathbf{w}_I + \mathbf{w}_P^H \mathbf{w}_P) \leq P, \\ & z(\mathbf{w}_I, \mathbf{w}_P, \rho) \geq \bar{z} \end{aligned} \quad (44)$$

Similarly, define $\mathbf{M} = \mathbf{h}^* \mathbf{h}^T$ and let 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 $M_{-n} = M_n^H$. Hence, 21 is transformed to 45. Introduce auxiliary variables

$$\begin{aligned} t'_{I/P,n} &= \mathbf{w}_{I/P}^H \mathbf{M}_n \mathbf{w}_{I/P} \\ &= \text{Tr}(\mathbf{M}_n \mathbf{w}_{I/P} \mathbf{w}_{I/P}^H) \\ &= \text{Tr}(\mathbf{M}_n \mathbf{W}_{I/P}) \end{aligned} \quad (46)$$

where $\mathbf{W}_{I/P} = \mathbf{w}_{I/P} \mathbf{w}_{I/P}^H$. Therefore, 45 rewrites as

$$\begin{aligned} z &= \frac{1}{2} k_2 \rho R_{\text{ant}} (t'_{I,0} + t'_{P,0}) \\ &\quad + \frac{3}{8} k_4 \rho^2 R_{\text{ant}}^2 \sum_{n=-N+1}^{N-1} 2t'_{I,n} t'_{I,n}^* + t'_{P,n} t'_{P,n}^* \\ &\quad + \frac{3}{2} k_4 \rho^2 R_{\text{ant}}^2 t'_{I,0} t'_{P,0} \end{aligned} \quad (47)$$

$$\begin{aligned} z &= \frac{1}{2} k_2 \rho R_{\text{ant}} (\mathbf{h}^H \mathbf{M}_{I,0} \mathbf{h} + \mathbf{h}^H \mathbf{M}_{P,0} \mathbf{h}) \\ &\quad + \frac{3}{8} k_4 \rho^2 R_{\text{ant}}^2 \sum_{n=-N+1}^{N-1} 2(\mathbf{h}^H \mathbf{M}_{I,n} \mathbf{h})(\mathbf{h}^H \mathbf{M}_{I,n} \mathbf{h})^* + (\mathbf{h}^H \mathbf{M}_{P,n} \mathbf{h})(\mathbf{h}^H \mathbf{M}_{P,n} \mathbf{h})^* \\ &\quad + \frac{3}{2} k_4 \rho^2 R_{\text{ant}}^2 (\mathbf{h}^H \mathbf{M}_{I,0} \mathbf{h})(\mathbf{h}^H \mathbf{M}_{P,0} \mathbf{h}) \end{aligned} \quad (37)$$

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

$$\begin{aligned} t'_{I/P,n}{}^{(k)}(t'_{I/P,n}{}^{(k)})^* &\approx 2\Re \left\{ t'_{I/P,n}{}^{(k)}(t'_{I/P,n}{}^{(k-1)})^* \right\} - t'_{I/P,n}{}^{(k-1)}(t'_{I/P,n}{}^{(k-1)})^* \\ &= 2\Re \left\{ \text{Tr}((t'_{I/P,n}{}^{(k-1)})^* \mathbf{M}_n \mathbf{W}_{I/P}^{(k)}) \right\} - t'_{I/P,n}{}^{(k-1)}(t'_{I/P,n}{}^{(k-1)})^* \\ &= \text{Tr} \left((t'_{I/P,n}{}^{(k-1)})^* \mathbf{M}_n \mathbf{W}_{I/P}^{(k)} \right) + \text{Tr}(t'_{I/P,n}{}^{(k-1)} \mathbf{M}_n^H \mathbf{W}_{I/P}^{(k)}) \\ &\quad - t'_{I/P,n}{}^{(k-1)}(t'_{I/P,n}{}^{(k-1)})^* \end{aligned} \quad (48)$$

and

$$\begin{aligned} t'_{I,0}{}^{(k)} t'_{P,0}{}^{(k)} &\approx t'_{I,0}{}^{(k)} t'_{P,0}{}^{(k-1)} + t'_{I,0}{}^{(k-1)} t'_{P,0}{}^{(k)} - t'_{I,0}{}^{(k-1)} t'_{P,0}{}^{(k-1)} \\ &= \text{Tr} \left(t'_{P,0}{}^{(k-1)} \mathbf{M}_0 \mathbf{W}_{I,0}^{(k)} \right) + \text{Tr}(t'_{I,0}{}^{(k-1)} \mathbf{M}_0^H \mathbf{W}_{P,0}^{(k)}) - t'_{I,0}{}^{(k-1)} t'_{P,0}{}^{(k-1)} \end{aligned} \quad (49)$$

Therefore, we have

$$\begin{aligned} \tilde{z}(\mathbf{W}_I^{(k)}, \mathbf{W}_P^{(k)}, \rho^{(k-1)}) &= \text{Tr}(\mathbf{A}_I^{(k)} \mathbf{W}_I^{(k)}) + \text{Tr}(\mathbf{A}_P^{(k)} \mathbf{W}_P^{(k)}) \\ &\quad - \frac{3k_4(\rho^{(k-1)})^2 R_{\text{ant}}^2}{8} \sum_{n=-N+1}^{N-1} 2t'_{I,n}{}^{(k-1)}(t'_{I,n}{}^{(k-1)})^* \\ &\quad - \frac{3k_4(\rho^{(k-1)})^2 R_{\text{ant}}^2}{2} t'_{I,0}{}^{(k-1)} t'_{P,0}{}^{(k-1)} \end{aligned} \quad (50)$$

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

$$\begin{aligned} \mathbf{A}_I^{(k)} &= \frac{k_2 \rho^{(k-1)} R_{\text{ant}}}{2} \mathbf{M}_0 \\ &\quad + \frac{3k_4(\rho^{(k-1)})^2 R_{\text{ant}}^2}{8} \sum_{n=-N+1}^{N-1} 2 \left((t'_{I,n}{}^{(k-1)})^* \mathbf{M}_n + t'_{I,n}{}^{(k-1)} \mathbf{M}_n^H \right) \\ &\quad + \frac{3k_4(\rho^{(k-1)})^2 R_{\text{ant}}^2}{2} t'_{P,0}{}^{(k-1)} \mathbf{M}_0 \end{aligned} \quad (51)$$

$$\begin{aligned} \mathbf{A}_P^{(k)} &= \frac{k_2 \rho^{(k-1)} R_{\text{ant}}}{2} \mathbf{M}_0 \\ &\quad + \frac{3k_4(\rho^{(k-1)})^2 R_{\text{ant}}^2}{8} \sum_{n=-N+1}^{N-1} (t'_{P,n}{}^{(k-1)})^* \mathbf{M}_n + t'_{P,n}{}^{(k-1)} \mathbf{M}_n^H \\ &\quad + \frac{3k_4(\rho^{(k-1)})^2 R_{\text{ant}}^2}{2} t'_{I,0}{}^{(k-1)} \mathbf{M}_0 \end{aligned} \quad (52)$$

Plug 50 into problem 44 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 .

Algorithm 2 Waveform Optimization

```

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 51 and 52
   6:   Obtain waveform matrices  $\mathbf{W}_{I/P}^{(k)}$  and  $\rho^{(k)}$  by solving problem 44
   7:   Update auxiliary  $t'_{I/P,n}{}^{(k)} \forall n$  by 46 for SCA
   8: until  $R^{(k)} - R^{(k-1)} \leq \epsilon$ 
   9: Generate CSCG random vectors  $\mathbf{r}_r \sim \mathcal{CN}(\mathbf{0}, \mathbf{I}_N) \forall r$ 
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  $\mathbf{w}_{I/P,r} = \mathbf{U} \mathbf{w}_{I/P}^* \Sigma^{\frac{1}{2}} \mathbf{r}_r \forall r$  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 44 and corresponding  $\mathbf{w}_{I,r}^*$ ,  $\mathbf{w}_{P,r}^*$ 
Output  $\mathbf{w}_I^*$ ,  $\mathbf{w}_P^*$ ,  $\rho^*$ 

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$$\begin{aligned} z &= \frac{1}{2} k_2 \rho R_{\text{ant}} (\mathbf{w}_I^H \mathbf{M}_0 \mathbf{w}_I + \mathbf{w}_P^H \mathbf{M}_0 \mathbf{w}_P) \\ &\quad + \frac{3}{8} k_4 \rho^2 R_{\text{ant}}^2 \sum_{n=-N+1}^{N-1} 2(\mathbf{w}_I^H \mathbf{M}_n \mathbf{w}_I)(\mathbf{w}_I^H \mathbf{M}_n \mathbf{w}_I)^* + (\mathbf{w}_P^H \mathbf{M}_n \mathbf{w}_P)(\mathbf{w}_P^H \mathbf{M}_n \mathbf{w}_P)^* \\ &\quad + \frac{3}{2} k_4 \rho^2 R_{\text{ant}}^2 (\mathbf{w}_I^H \mathbf{M}_0 \mathbf{w}_I)(\mathbf{w}_P^H \mathbf{M}_0 \mathbf{w}_P) \end{aligned} \quad (45)$$