***Abstract*—Simultaneous Wireless Information and Power Transfer (SWIPT) is limited by the low power level of the receive Radio-Frequency (RF) signal. To tackle this problem, we introduce Intelligent Reflecting Surface (IRS) that brings a high passive beamforming gain by adjusting reflecting elements, which compensates the propagation loss and boosts the energy efficiency with low power consumption. This paper investigates an IRS-aided multiuser Orthogonal Frequency Division Multiplexing (OFDM) SWIPT system based on practical nonlinear harvester model, where the single-antenna Access Point (AP) transmits information and energy simultaneously to multiple single-antenna users under the assist of IRS. We aim to maximize the weighted sum Rate-Energy (R-E) region via jointly optimizing the transmit waveform at the AP, the phase shifts at the IRS, and the power splitting ratio at all users. The problem is transformed to a current maximization problem subject to rate constraint, and we propose an low-complexity alternating algorithm to obtain suboptimal solutions iteratively. Simulation results demonstrated significant R-E region enlargement over benchmark schemes when IRS is properly configured.**

I. Introduction

A. Simultaneous Wireless Information and Power Transfer

With the great advance in communication performance (throughput, latency, outage), the main challenge of wireless network has come to energy supply. Most existing mobile devices are powered by batteries that require frequent charging or replacement, which leads to high maintenance cost and thus restricts the scale of networks. Although solar energy and inductive coupling has become popular alternatives, the former depends on the environment while the latter has a very short operation range. Simultaneous Wireless Information and Power Transfer (SWIPT) is a promising solution to connect and power mobile devices via electromagnetic (EM) waves in the Radio-Frequency (RF) band. It provides low power (in μW level) but broad coverage (up to hundreds of meters) [1] in a sustainable and controllable manner. The decreasing trend in electronic power consumption also boosts the paradigm shift from dedicated power source to Wireless Power Transfer (WPT) and SWIPT.

The concept of SWIPT were first cast in [2], where the authors investigated the Rate-Energy (R-E) tradeoff for a flat Gaussian channel and some discrete channels. Two practical receiver structures were then proposed in [3], namely Time Switching (TS) that switches between energy harvesting (EH) and Information Decoding (ID) modes, and Power Splitting (PS) that splits the received signal into individual components. On top of this, [4] characterized the R-E region for a Multiple-Input Multiple-Output (MIMO) broadcast system under TS and PS setup. Information and power beamforming was then considered in multi-user multi-input single-output (MISO) systems to maximize the Weighted Sum-Power (WSP) subjective to Signal-to-Interference-plus-Noise Ratio (SINR) constraints [5]. Motivated by this, [6] investigated fundamental transceiver modules, information and power scheduling, and interference management for SWIPT systems. However, [7] pointed out that the Radio Frequency (RF)-to-Direct Current (DC) conversion efficiency depends on the harvester input power level, which also suggested a parametric harvester model based on curve fitting and proposed an iterative resource allocation algorithm. From another perspective, [8], [9] demonstrated that multisine waveform is more suitable for WPT as it outperforms single tone in both operation range and RF-to-DC efficiency. [10] derived a tractable nonlinear harvester model based on the Taylor expansion of diode I-V characteristics and proposed an adaptive waveform optimization algorithm to maximize the output DC current under rate constraints. Simulation and experiments demonstrated the benefit of modelling rectifier nonlinearity in system design [11], [12]. The work was extended to SWIPT in [13] where a superposition of modulated information waveform and multisine power waveform is optimized to enlarge the R-E region. In contrast, [14] suggested an adaptive dual-mode SWIPT, which alternates between single-tone transmission that exploits conventional modulation for high-rate applications and multisine transmission that encodes the information in the Peak-to-Average Ratio (PAPR) for power-demanding applications. By assuming On-Off-Keying (OOK) where bit 1 carries energy, [15] compared unary and Run-Length-Limited (RLL) code in terms of rate vs battery overflow/underflow probability, and adapted conventional modulation schemes to ensure WPT is only activated at the points with large offset. Also, a learning approach [16] demonstrated that the offset of the power symbol is positively correlated to the harvester energy constraint, while the information symbols are symmetrically distributed around the origin. It confirmed that the superposed waveform is feasible to enlarge R-E region when considering rectifier nonlinearity. SWIPT was also explored in the network design. [17] proposed a cooperative SWIPT Non-Orthogonal Multiple Access (NOMA) protocol with three user selection schemes such that the strong user assists the EH of the weak user. In [18], SWIPT based on Rate Splitting (RS) was formulated as a Weighted Sum-Rate (WSR) maximization problem subject to total harvested energy constraint for separated Information Receivers (IRs) and Energy Receivers (ERs).

B. Intelligent Reflecting Surface

Intelligent Reflecting Surface (IRS) adapts the wireless environment to increase spectrum and energy efficiency. In practice, an IRS consists of multiple individual reflecting elements that adjust the amplitude and phase of the incident signal through passive beamforming. Different from relay and backscatter communication, IRS assists the primary transmission without any active components, leading to low power consumption and no thermal noise added to the reflected signal. Compared with the linear increase in Amplify-and-Forward (AF) relay, the received power scales quadratically with the number of reflectors [19], which can be interpreted as a Maximum Ratio Combining (MRC) superposed to a Maximum Ratio Transmission (MRT).

Inspired by the advance in real-time reconfigurable metamaterials [20], [21] introduced a programmable metasurface that steers or polarizes the EM wave at specific frequency to mitigate path loss and multi-path fading. At the same time, [22] constructed an adjustable reflect array that ensures reliable millimeter-wave (mmWave) communication based on a beam-searching algorithm to reduce indoor signal blockage. Motivated by this, [23], [19] introduced an IRS-assisted MISO system and proposed a beamforming algorithm that jointly optimizes the precoder at the Access Point (AP) and the phase shifts at the IRS to maximize Signal-to-Noise Ratio (SNR). The active and passive beamforming problem was extended to the discrete phase shift case [24] and the multiuser case [25]. In [26], channel estimation for Time Division Duplex (TDD) systems was carried through a two-stage Minimum Mean Squared Error (MMSE)-based protocol that sequentially estimates the cascaded channel of each IRS element with the others switched off. Starting from the impedance equation, [27] investigated the influence of phase shift on the reflection amplitude and proposed a parametric IRS model via curve fitting. Recent research also explored the opportunity of integrating IRS with Orthogonal Frequency Division Multiplexing (OFDM) systems. [28] exploited spatial correlation to reduce estimation overhead and design complexity by assuming adjacent elements share a common reflection coefficient. On top of this, group-based OFDM channel estimation was investigated in [29]. By adjusting IRS over time slots, [30] introduced artificial diversity within coherence time and investigated resource allocation and IRS configuration per Resource Block (RB). Real-time high-definition video transmission was performed over a prototype constructed with Positive Intrinsic-Negative (PIN) diodes, which demonstrated the feasibility and benefit of IRS at GHz and mmWave frequency [31].

C. IRS-aided SWIPT

The effective channel enhancement and low power consumption of IRS are expected to bring more opportunities to SWIPT. Assuming linear harvester model with energy interference, [32] proved that at most one energy beam is required to maximize the WSP subject to SINR constraints. The fairness issue was then considered in [33], which maximize the minimum output power based on Alternating Optimization (AO) and Semi-Definite Relaxation (SDR) techniques based on perfect energy interference cancellation. [34] proposed a novel penalty-based algorithm, whose inner layer employs Block Coordinate Descent (BCD) method to update precoders, phase shifts and auxiliary variables while the outer layer updates the penalty coefficients. It demonstrated that Line-of-Sight (LoS) links can boost the harvested power since the rank-deficient channels are highly correlated such that a single energy stream can satisfy the energy constraints of all ERs. In [35], the WSR maximization of MIMO SWIPT was first transformed to Weighted Minimum Mean Square Error (WMMSE) problem then solved by BCD with low-complexity iterative algorithms. However, most existing IRS-SWIPT papers focus on narrow-band transmission over linear harvester model.

D. Research Proposal

In this paper, we consider an IRS-aided multiuser (Single-Input Single-Output) SISO OFDM SWIPT system based on practical nonlinear harvester model.

II. System Model

Consider an IRS-aided multiuser SISO OFDM SWIPT system where the IRS assists the information and energy transmission of all users. 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 ($n = 1, \dots, N$). Suppose each subband is allocated to one user per time slot. It is assumed that the IRS performs channel estimation in the first subframe and supports information and power transfer in the second subframe [29]. 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 [36], [5]. Since passive FSS is not reconfigurable with fixed physical characteristics [37], 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 [10] and creates no interference to the information signal [38], 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 [4], 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 $(1 - \lambda)$ and λ respectively. Hence, the achievable rate-energy region can be obtained through a time sharing between wireless power transfer (WPT) with $\lambda = 1$ and wireless information transfer (WIT) with $\lambda = 0$. The adjustment of λ 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

Denote $\tilde{x}_{I,n}(t)$ as the information symbol transmitted over subband n, which belongs to one user at time t and follows a capacity-achieving i.i.d. Circular Symmetric Complex Gaussian (CSCG) distribution $\tilde{x}_{I,n} \sim \mathcal{CN}(0, 1)$. Let $\alpha_{k,n}$ be the allocation indicator, namely if subband n is given to user k ($k = 1, \dots, K$), we have $\alpha_{k,n} = 1$ and $\alpha_{k',n} = 0 \, \forall k' \neq k$. Let

$\boldsymbol{\alpha}_k = [\alpha_{k,1}, \ldots, \alpha_{k,N}]^T \in \mathbb{C}^{N\times1}$. The superposed transmit signal at time t is

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

where $w_{I/P,n} = s_{I/P,n}e^{j\psi_{I/P,n}}$ collects the magnitude and phase of the information and power signal at frequency n. We further define the waveform vectors $\boldsymbol{w}_{I/P} = [w_{I/P,1}, \ldots, w_{I/P,N}]^T \in \mathbb{C}^{N\times1}$.

B. Composite Channel Model

Denote the frequency response of the AP-user k direct link as $\boldsymbol{h}_{D,k} = [h_{D,k,1}, \ldots, h_{D,k,N}]^T \in \mathbb{C}^{N\times1}$. Let $[\boldsymbol{h}_{I,1}, \ldots, \boldsymbol{h}_{I,N}] \in \mathbb{C}^{L\times N}$ be the frequency response of AP-IRS incident channel, where $\boldsymbol{h}_{I,n} \in \mathbb{C}^{L\times1}$ corresponds to the n-th incident channel. Similarly, let $[\boldsymbol{h}_{R,k,1}, \ldots, \boldsymbol{h}_{R,k,N}]^H \in \mathbb{C}^{N\times L}$ be the frequency response of IRS-user k reflective channel, where $\boldsymbol{h}_{R,k,n}^H \in \mathbb{C}^{1\times L}$ corresponds to the n-th reflective channel. At the IRS, element l ($l = 1, \ldots, L$) redistributes the received signal by adjusting the amplitude reflection coefficient $\beta_l \in [0, 1]$ and phase shift $\theta_l \in [0, 2\pi)$ [1]. On top of this, the IRS matrix is constructed by collecting the reflection coefficients onto the main diagonal entries as $\boldsymbol{\Theta} = \mathrm{diag}\left\{\beta_1 e^{j\theta_1}, \ldots, \beta_L e^{j\theta_L}\right\} \in \mathbb{C}^{L\times L}$. 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

$$h_{E,k,n} = \boldsymbol{h}_{R,k,n}^H \boldsymbol{\Theta} \boldsymbol{h}_{I,n} = \boldsymbol{v}_{k,n}^H \boldsymbol{\phi} \quad (2)$$

where $\boldsymbol{v}_{k,n}^H = \boldsymbol{h}_{R,k,n}^H \mathrm{diag}(\boldsymbol{h}_{I,n}) \in \mathbb{C}^{1\times L}$ and $\boldsymbol{\phi} = [e^{j\theta_1}, \ldots, e^{j\theta_L}] \in \mathbb{C}^{L\times1}$. Both direct and extra link contributes to the corresponding composite channel as

$$h_{k,n} = A_{k,n}e^{j\bar{\psi}_{k,n}} = h_{D,k,n} + \boldsymbol{v}_{k,n}^H \boldsymbol{\phi} \quad (3)$$

where $A_{k,n}$ and $\bar{\psi}_{k,n}$ are the amplitude and phase of the composite channel of user k at subband n. Let $\boldsymbol{V}_k^H = [\boldsymbol{v}_{k,1}, \ldots, \boldsymbol{v}_{k,N}]^H \in \mathbb{C}^{N\times L}$, the extra link for user k is $\boldsymbol{h}_{E,k} = [h_{E,k,1}, \ldots, h_{E,k,N}]^T = \boldsymbol{V}_k^H \boldsymbol{\phi} \in \mathbb{C}^{N\times1}$. Therefore, the composite channel of user k is

$$\boldsymbol{h}_k = \boldsymbol{h}_{D,k} + \boldsymbol{V}_k^H \boldsymbol{\phi} \quad (4)$$

C. Receive Signal

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

$$y_k(t) = \Re\left\{\sum_{n=1}^{N} h_{k,n}\left(w_{I,n}\tilde{x}_{I,n}(t) + w_{P,n}\right) e^{j2\pi f_n t}\right\} \quad (5)$$

[1]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 $[0, 2\pi)$.

which can be divided into

$$y_{I,k}(t) = \Re\left\{\sum_{n=1}^{N} h_{k,n} w_{I,n}\tilde{x}_{I,n}(t) e^{j2\pi f_n t}\right\} \quad (6)$$

$$y_{P,k}(t) = \Re\left\{\sum_{n=1}^{N} h_{k,n} w_{P,n} e^{j2\pi f_n t}\right\} \quad (7)$$

D. Information Decoder

A 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

$$R_k(\boldsymbol{w}_I, \boldsymbol{\phi}, \rho, \boldsymbol{\alpha}_k) = \sum_{n=1}^{N} \alpha_{k,n} \log_2\left(1 + \frac{(1-\rho)|h_{k,n}w_{I,n}|^2}{\sigma_n^2}\right) \quad (8)$$

where σ_n^2 is the variance of the noise at RF band and during RF-to-BB conversion on tone n. Rate 8 is achievable with either waveform cancellation or translated demodulation [38].

E. Energy Harvester

Consider a nonlinear diode model based on the Taylor expansion of a small signal model [10], [38], which highlights the dependency of harvester output DC current on the received waveform of user k as

$$i_k(\boldsymbol{w}_I, \boldsymbol{w}_P, \boldsymbol{\phi}, \rho) \approx \sum_{i=0}^{\infty} k_i' \rho^{i/2} R_{\text{ant}}^{i/2} \mathcal{E}\left\{\mathcal{A}\left\{y_k(t)^i\right\}\right\} \quad (9)$$

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 $i = 1, \ldots, \infty$, i_s is saturation current, n is diode ideality factor, v_t is thermal voltage. For a fixed channel and waveform, $\mathcal{A}\{.\}$ extracts the DC component of the received signal while $\mathcal{E}\{.\}$ covers the expectation over $\tilde{x}_{I,n}$.

With the assumption of evenly spaced frequencies, we have $\mathcal{E}\left\{y_k(t)^i\right\} = 0$ $\forall i$ 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 9 is equivalent to maximizing a monotonic function [10]

$$z_k(\boldsymbol{w}_I, \boldsymbol{w}_P, \boldsymbol{\phi}, \rho) = \sum_{i\,\text{even}, i\geq2}^{n_0} k_i \rho^{i/2} R_{\text{ant}}^{i/2} \mathcal{E}\left\{\mathcal{A}\left\{y_k(t)^i\right\}\right\} \quad (10)$$

where $k_i = i_s/i!(nv_t)^i$. We choose $n_0 = 4$ to investigate the fundamental impact of diode nonlinearity on waveform design. Note that $\mathcal{E}\left\{|\tilde{x}_{I,n}|^2\right\} = 1$ and $\mathcal{E}\left\{|\tilde{x}_{I,n}|^4\right\} = 2$, which can be interpreted as a modulation gain on the nonlinear terms of the output DC current.

For simplicity, we define $\boldsymbol{W}_{I/P} = \boldsymbol{w}_{I/P}\boldsymbol{w}_{I/P}^H$ and $\boldsymbol{H}_k = \boldsymbol{h}_k\boldsymbol{h}_k^H$ as waveform matrices and channel matrix of user k. Let $\boldsymbol{W}_{I/P,n}$, $\boldsymbol{H}_{k,n}$ keep the n-th ($n = -N+1, \ldots, N-1$) diagonal of $\boldsymbol{W}_{I/P}$, $\boldsymbol{H}_k$ and null the remaining entries, respectively. Due to the positive definiteness of $\boldsymbol{W}_{I/P}$ and $\boldsymbol{H}_k$, we have $\boldsymbol{W}_{I/P,-n} = \boldsymbol{W}_{I/P,n}^H$ and $\boldsymbol{H}_{k,-n} = \boldsymbol{H}_{k,n}^H$. Let $\beta_2 = k_2 R_{\text{ant}}$ and $\beta_4 = k_4 R_{\text{ant}}^2$. On top of this, nonzero terms in 10 are detailed in 11 – 18 such that the current expression reduces to 19 – 21.

F. Weighted Sum Rate-Energy Region

Define the achievable weighted sum rate-energy (WSR-E) region as

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

where P is the transmit power budget and $u_{I,k}, u_{P,k}$ are the information and power weight of user k.

III. Single-User Optimization

Consider a single-user waveform and IRS optimization problem where $\boldsymbol{\alpha} = \mathbf{1}^{N\times 1}$. We characterize the rate-energy region through a current maximization problem subject to transmit power, rate, and IRS constraints

$$\max_{\boldsymbol{w}_I, \boldsymbol{w}_P, \boldsymbol{\phi}, \rho} \quad z(\boldsymbol{w}_I, \boldsymbol{w}_P, \boldsymbol{\phi}, \rho) \tag{23a}$$

$$\text{s.t.} \quad \frac{1}{2}(\boldsymbol{w}_I^H \boldsymbol{w}_I + \boldsymbol{w}_P^H \boldsymbol{w}_P) \leq P, \tag{23b}$$

$$\sum_n \log_2 \left(1 + \frac{(1-\rho)|(h_{D,n} + \boldsymbol{v}_n^H \boldsymbol{\phi}) w_{I,n}|^2}{\sigma_n^2} \right) \geq \bar{R}, \tag{23c}$$

$$|\phi_l| = 1, \quad l = 1, \ldots, L, \tag{23d}$$

$$0 \leq \rho \leq 1 \tag{23e}$$

Problem 23 is intricate due to the non-convex objective function with coupled variables. To reduce the design complexity, we propose an suboptimal alternating optimization algorithm

$$\mathcal{E}\left\{\mathcal{A}\left\{y_{I,k}^2(t)\right\}\right\} = \frac{1}{2}\sum_n (h_{k,n} w_{I,n})(h_{k,n} w_{I,n})^* \tag{11}$$

$$= \frac{1}{2}\boldsymbol{h}_k^H \boldsymbol{W}_{I,0}^* \boldsymbol{h}_k = \frac{1}{2}\boldsymbol{w}_I^H \boldsymbol{H}_{k,0}^* \boldsymbol{w}_I \tag{12}$$

$$\mathcal{E}\left\{\mathcal{A}\left\{y_{I,k}^4(t)\right\}\right\} = \frac{3}{4}\left(\sum_n (h_{k,n} w_{I,n})(h_{k,n} w_{I,n})^*\right)^2 \tag{13}$$

$$= \frac{3}{4}(\boldsymbol{h}_k^H \boldsymbol{W}_{I,0}^* \boldsymbol{h}_k)^2 = \frac{3}{4}(\boldsymbol{w}_I^H \boldsymbol{H}_{k,0}^* \boldsymbol{w}_I)^2 \tag{14}$$

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

$$= \frac{1}{2}\boldsymbol{h}_k^H \boldsymbol{W}_{P,0}^* \boldsymbol{h}_k = \frac{1}{2}\boldsymbol{w}_P^H \boldsymbol{H}_{k,0}^* \boldsymbol{w}_P \tag{16}$$

$$\mathcal{A}\left\{y_{P,k}^4(t)\right\} = \frac{3}{8}\sum_{\substack{n_1,n_2,n_3,n_4 \\ n_1+n_2=n_3+n_4}} (h_{k,n_1} w_{P,n_1})(h_{k,n_2} w_{P,n_2})(h_{k,n_3} w_{P,n_3})^*(h_{k,n_4} w_{P,n_4})^* \tag{17}$$

$$= \frac{3}{8}\sum_{n=-N+1}^{N-1} (\boldsymbol{h}_k^H \boldsymbol{W}_{P,n}^* \boldsymbol{h}_k)(\boldsymbol{h}_k^H \boldsymbol{W}_{P,n}^* \boldsymbol{h}_k)^* = \frac{3}{8}\sum_{n=-N+1}^{N-1} (\boldsymbol{w}_P^H \boldsymbol{H}_{k,n}^* \boldsymbol{w}_P)(\boldsymbol{w}_P^H \boldsymbol{H}_{k,n}^* \boldsymbol{w}_P)^* \tag{18}$$

$$z_k(\boldsymbol{w}_I, \boldsymbol{w}_P, \boldsymbol{\phi}, \rho) = \beta_2 \rho \left(\mathcal{E}\left\{\mathcal{A}\left\{y_{I,k}^2(t)\right\}\right\} + \mathcal{A}\left\{y_{P,k}^2(t)\right\}\right) + \beta_4 \rho^2 \left(\mathcal{E}\left\{\mathcal{A}\left\{y_{I,k}^4(t)\right\}\right\} + \mathcal{A}\left\{y_{P,k}^4(t)\right\} + 6\mathcal{E}\left\{\mathcal{A}\left\{y_{I,k}^2(t)\right\}\right\}\mathcal{A}\left\{y_{P,k}^2(t)\right\}\right) \tag{19}$$

$$\begin{aligned} = &\frac{1}{2}\beta_2 \rho (\boldsymbol{h}_k^H \boldsymbol{W}_{I,0}^* \boldsymbol{h}_k + \boldsymbol{h}_k^H \boldsymbol{W}_{P,0}^* \boldsymbol{h}_k) \\ &+ \frac{3}{8}\beta_4 \rho^2 \left(2(\boldsymbol{h}_k^H \boldsymbol{W}_{I,0}^* \boldsymbol{h}_k)^2 + \sum_{n=-N+1}^{N-1} (\boldsymbol{h}_k^H \boldsymbol{W}_{P,n}^* \boldsymbol{h}_k)(\boldsymbol{h}_k^H \boldsymbol{W}_{P,n}^* \boldsymbol{h}_k)^*\right) \\ &+ \frac{3}{2}\beta_4 \rho^2 (\boldsymbol{h}_k^H \boldsymbol{W}_{I,0}^* \boldsymbol{h}_k)(\boldsymbol{h}_k^H \boldsymbol{W}_{P,0}^* \boldsymbol{h}_k) \end{aligned} \tag{20}$$

$$\begin{aligned} = &\frac{1}{2}\beta_2 \rho (\boldsymbol{w}_I^H \boldsymbol{H}_{k,0}^* \boldsymbol{w}_I + \boldsymbol{w}_P^H \boldsymbol{H}_{k,0}^* \boldsymbol{w}_P) \\ &+ \frac{3}{8}\beta_4 \rho^2 \left(2(\boldsymbol{w}_I^H \boldsymbol{H}_{k,0}^* \boldsymbol{w}_I)^2 + \sum_{n=-N+1}^{N-1} (\boldsymbol{w}_P^H \boldsymbol{H}_{k,n}^* \boldsymbol{w}_P)(\boldsymbol{w}_P^H \boldsymbol{H}_{k,n}^* \boldsymbol{w}_P)^*\right) \\ &+ \frac{3}{2}\beta_4 \rho^2 (\boldsymbol{w}_I^H \boldsymbol{H}_{k,0}^* \boldsymbol{w}_I)(\boldsymbol{w}_P^H \boldsymbol{H}_{k,0}^* \boldsymbol{w}_P) \end{aligned} \tag{21}$$

that iteratively updates the IRS phase shift, transmit waveform, and receive power splitting ratio iteratively.

A. IRS Phase Shift

1) Frequency-Selective IRS: Each element in frequency-selective IRS is expected to provide subband-dependent reflection coefficients. Hence, $\boldsymbol{\phi}_n$ replaces $\boldsymbol{\phi}$ in 23 and the IRS has a total degree of freedom (DoF) of NL. Note that $|(h_{D,n} + \boldsymbol{v}_n^H \boldsymbol{\phi}_n) w_{I,n}| \leq |h_{D,n} w_{I,n}| + |\boldsymbol{v}_n^H \boldsymbol{\phi}_n w_{I,n}|$ where the equality holds when the direct and IRS-aided links are aligned. Therefore, we choose the phase shift of element l at subband n as

$$\theta_{n,l}^\star = \angle h_{D,n} - \angle h_{R,n,l} - \angle h_{I,n,l} \tag{24}$$

That is to say, the optimal phase shift is obtained in closed form in the single-user scenario, and the phase of the composite channel equals that of the direct channel.

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

$$\begin{aligned} |h_{D,n} + \boldsymbol{v}_n^H \boldsymbol{\phi}|^2 &= |h_{D,n}|^2 + h_{D,n}^* \boldsymbol{v}_n^H \boldsymbol{\phi} + \boldsymbol{\phi}^H \boldsymbol{v}_n h_{D,n} + \boldsymbol{\phi}^H \boldsymbol{v}\boldsymbol{v}^H \boldsymbol{\phi} \\ &= \bar{\boldsymbol{\phi}}^H \boldsymbol{R}_n \bar{\boldsymbol{\phi}} = \mathrm{Tr}(\boldsymbol{R}_n \bar{\boldsymbol{\phi}} \bar{\boldsymbol{\phi}}^H) = \mathrm{Tr}(\boldsymbol{R}_n \boldsymbol{\Phi}) \end{aligned} \tag{25}$$

where t is an auxiliary variable with unit modulus and

$$\boldsymbol{R}_n = \begin{bmatrix} \boldsymbol{v}_n \boldsymbol{v}_n^H & \boldsymbol{v}_n h_{D,n} \\ h_{D,n}^* \boldsymbol{v}_n^H & h_{D,n}^* h_{D,n} \end{bmatrix}, \quad \bar{\boldsymbol{\phi}} = \begin{bmatrix} \boldsymbol{\phi} \\ t \end{bmatrix}, \quad \boldsymbol{\Phi} = \bar{\boldsymbol{\phi}} \bar{\boldsymbol{\phi}}^H \tag{26}$$

with $\boldsymbol{R}_n, \boldsymbol{\Phi} \in \mathbb{C}^{(L+1)\times(L+1)}$ and $\bar{\boldsymbol{\phi}} \in \mathbb{C}^{(L+1)\times 1}$. On top of this, the outer product of composite channel rewrites as

$$\boldsymbol{h}\boldsymbol{h}^H = \boldsymbol{M}^H \boldsymbol{\Phi} \boldsymbol{M} \tag{27}$$

where $\boldsymbol{M} = [\boldsymbol{V}^H, \boldsymbol{h}_D]^H \in \mathbb{C}^{(L+1)\times N}$.

The phase optimization subproblem is formed as follows. With a given waveform $\boldsymbol{w}_I, \boldsymbol{w}_P, \rho$, introduce auxiliary variables

$$\begin{aligned} t_{I/P,n} &= \boldsymbol{h}^H \boldsymbol{W}_{I/P,n}^* \boldsymbol{h} \\ &= \mathrm{Tr}(\boldsymbol{h}\boldsymbol{h}^H \boldsymbol{W}_{I/P,n}^*) \\ &= \mathrm{Tr}(\boldsymbol{M}^H \boldsymbol{\Phi} \boldsymbol{M} \boldsymbol{W}_{I/P,n}^*) \\ &= \mathrm{Tr}(\boldsymbol{M} \boldsymbol{W}_{I/P,n}^* \boldsymbol{M}^H \boldsymbol{\Phi}) \\ &= \mathrm{Tr}(\boldsymbol{C}_{I/P,n} \boldsymbol{\Phi}) \end{aligned} \tag{28}$$

where we define

$$\boldsymbol{C}_{I/P,n} = \boldsymbol{M} \boldsymbol{W}_{I/P,n}^* \boldsymbol{M}^H \in \mathbb{C}^{(L+1)\times(L+1)} \tag{29}$$

Therefore, 20 rewrites as

$$\begin{aligned} z(\boldsymbol{\Phi}) &= \frac{1}{2}\beta_2 \rho (t_{I,0} + t_{P,0}) \\ &\quad + \frac{3}{8}\beta_4 \rho^2 \left(2t_{I,0}^2 + \sum_{n=-N+1}^{N-1} t_{P,n} t_{P,n}^* \right) \\ &\quad + \frac{3}{2}\beta_4 \rho^2 t_{I,0} t_{P,0} \end{aligned} \tag{30}$$

We use first-order Taylor expansion to approximate the second-order terms in 30. Based on the variables optimized at iteration $i-1$, the local approximation at iteration i suggests [39]

$$(t_{I,0}^{(i)})^2 \geq 2t_{I,0}^{(i)} t_{I,0}^{(i-1)} - (t_{I,0}^{(i-1)})^2 \tag{31}$$

$$t_{P,n}^{(i)} (t_{P,n}^{(i)})^* \geq 2\Re\left\{ t_{P,n}^{(i)} (t_{P,n}^{(i-1)})^* \right\} - t_{P,n}^{(i-1)} (t_{P,n}^{(i-1)})^* \tag{32}$$

$$\begin{aligned} t_{I,0}^{(i)} t_{P,0}^{(i)} &= \frac{1}{4}(t_{I,0}^{(i)} + t_{P,0}^{(i)})^2 - \frac{1}{4}(t_{I,0}^{(i)} - t_{P,0}^{(i)})^2 \\ &\geq \frac{1}{2}(t_{I,0}^{(i)} + t_{P,0}^{(i)})(t_{I,0}^{(i-1)} + t_{P,0}^{(i-1)}) \\ &\quad - \frac{1}{4}(t_{I,0}^{(i-1)} + t_{P,0}^{(i-1)})^2 - \frac{1}{4}(t_{I,0}^{(i)} - t_{P,0}^{(i)})^2 \end{aligned} \tag{33}$$

31 – 33 provide lower bounds to corresponding terms such that the approximated current function at iteration i is given in 34. Hence, problem 23 is transformed to

$$\max_{\boldsymbol{\Phi}} \quad \tilde{z}(\boldsymbol{\Phi}) \tag{35a}$$

$$\text{s.t.} \quad \sum_n \log_2 \left(1 + \frac{(1-\rho)|w_{I,n}|^2 \mathrm{Tr}(\boldsymbol{R}_n \boldsymbol{\Phi})}{\sigma_n^2} \right) \geq \bar{R}, \tag{35b}$$

$$\boldsymbol{\Phi}_{l,l} = 1, \quad l = 1, \ldots, L+1, \tag{35c}$$

$$\boldsymbol{\Phi} \succeq 0, \tag{35d}$$

$$\mathrm{rank}(\boldsymbol{\Phi}) = 1 \tag{35e}$$

We then relax the rank constraint 35e and solve the optimal IRS matrix $\boldsymbol{\Phi}^\star$ iteratively by interior-point method. If $\mathrm{rank}(\boldsymbol{\Phi}^\star) = 1$, the optimal phase shift vector $\bar{\boldsymbol{\phi}}^\star$ is attained by eigenvalue decomposition (EVD). Otherwise, a best feasible candidate $\bar{\boldsymbol{\phi}}^\star$ can be extracted through Gaussian randomization method [40]. First, perform EVD on $\boldsymbol{\Phi}^\star$ as $\boldsymbol{\Phi}^\star = \boldsymbol{U}_{\boldsymbol{\Phi}^\star} \boldsymbol{\Sigma}_{\boldsymbol{\Phi}^\star} \boldsymbol{U}_{\boldsymbol{\Phi}^\star}^H$. Then, we generate Q CSCG random vectors $\boldsymbol{r}_q \sim \mathcal{CN}(\boldsymbol{0}, \boldsymbol{I}_{L+1}),\ q = 1, \ldots, Q$ and construct the corresponding candidates $\bar{\boldsymbol{\phi}}_q = e^{j \arg\left(\boldsymbol{U}_{\boldsymbol{\Phi}^\star} \boldsymbol{\Sigma}_{\boldsymbol{\Phi}^\star}^{\frac{1}{2}} \boldsymbol{r}_q \right)}$. Next, the optimal solution $\bar{\boldsymbol{\phi}}^\star$ is approximated by the one achieving maximum objective value 35a. Finally, we can retrieve the phase shift by $\theta_l = \arg(\phi_l^\star / \phi_{L+1}^\star),\ l = 1, \ldots, L$. The algorithm for the phase shift optimization subproblem is summarized in Algorithm 1.

B. Waveform and Splitting Ratio

1) Geometric Programming: Following [38], it can be observed from 8 and 19 that the optimal phases of information and power waveform are both match to the composite channel as

$$\psi_{I,n}^\star = \psi_{P,n}^\star = -\bar{\psi}_n \tag{36}$$

By such a phase selection, we have

$$|(h_{D,n} + \boldsymbol{v}_n^H \boldsymbol{\phi}_n) w_{I,n}| = |h_{D,n}||w_{I,n}| + |\boldsymbol{v}_n^H \boldsymbol{\phi}_n||w_{I,n}| \tag{37}$$

Also, denote the waveform amplitude at subband n as

$$s_{I/P,n} = |w_{I/P,n}| e^{j\psi_{I/P,n}} \tag{38}$$

Algorithm 1 FF-IRS: Phase Shift

Input $\beta_2, \beta_4, \boldsymbol{h}_D, \boldsymbol{h}_I, \boldsymbol{h}_R, Q, \bar{R}, \epsilon, \rho, \boldsymbol{w}_{I/P}, \sigma_n\ \forall n$ by 26, 29
Initialize $i \leftarrow 0, \boldsymbol{\Phi}^{(0)}, t_{I/P,n}^{(0)}\ \forall n$ by 28
Construct $\boldsymbol{M}, \boldsymbol{R}_n, \boldsymbol{C}_{I/P,n}\ \forall n$ by 27, 26, 29
repeat
  $i \leftarrow i+1$
  Obtain IRS matrix $\boldsymbol{\Phi}^{(i)}$ by solving problem 35
  Update auxiliary $t_{I/P,n}^{(i)} \forall n$ by 28 for SCA
until $|(z^{(i)} - z^{(i-1)})/z^{(i)}| \leq \epsilon$
Perform EVD $\boldsymbol{\Phi}^\star = \boldsymbol{U}_{\boldsymbol{\Phi}^\star}\boldsymbol{\Sigma}_{\boldsymbol{\Phi}^\star}\boldsymbol{U}_{\boldsymbol{\Phi}^\star}^H$
Generate random vectors $\boldsymbol{r}_q \sim \mathcal{CN}(\boldsymbol{0}, \boldsymbol{I}_{L+1})\ \forall q$
Construct candidate IRS vectors $\bar{\boldsymbol{\phi}}_q = e^{j\arg\left(\boldsymbol{U}_{\boldsymbol{\Phi}^\star}\boldsymbol{\Sigma}_{\boldsymbol{\Phi}^\star}^{\frac{1}{2}}\boldsymbol{r}_q\right)}$ and matrices $\boldsymbol{\Phi}_q = \bar{\boldsymbol{\phi}}_q\bar{\boldsymbol{\phi}}_q^H\ \forall q$
Select best solution $\boldsymbol{\Phi}^\star$ and $\boldsymbol{\phi}^\star$ for problem 35
Compute phase shift by $\theta_l^\star = \arg(\phi_l^\star/\phi_{L+1}^\star),\ l = 1,\ldots,L$
Output $\theta_l^\star\ \forall l$

which is further collected into $\boldsymbol{s}_{I/P} \in \mathbb{C}^{N\times 1}$. Therefore, the original problem 23 is reduced to an amplitude optimization problem

$$\max_{\boldsymbol{s}_I, \boldsymbol{s}_P, \rho} \quad z(\boldsymbol{s}_I, \boldsymbol{s}_P, \rho) \tag{39a}$$

$$\text{s.t.} \quad \frac{1}{2}(\boldsymbol{s}_I^H\boldsymbol{s}_I + \boldsymbol{s}_P^H\boldsymbol{s}_P) \leq P, \tag{39b}$$

$$\sum_n \log_2\left(1 + \frac{(1-\rho)A_n^2 s_{I,n}^2}{\sigma_n^2}\right) \geq \bar{R} \tag{39c}$$

with z given by 40. We introduce an auxiliary variable t'' and transform problem 39 into

$$\min_{\boldsymbol{s}_I, \boldsymbol{s}_P, \rho, t''} \quad \frac{1}{t''} \tag{41a}$$

$$\text{s.t.} \quad \frac{1}{2}(\boldsymbol{s}_I^H\boldsymbol{s}_I + \boldsymbol{s}_P^H\boldsymbol{s}_P) \leq P, \tag{41b}$$

$$\frac{t''}{z(\boldsymbol{s}_I, \boldsymbol{s}_P, \rho)} \leq 1, \tag{41c}$$

$$\frac{2^{\bar{R}}}{\prod_n\left(1 + \frac{(1-\rho)A_n^2 s_{I,n}^2}{\sigma_n^2}\right)} \leq 1 \tag{41d}$$

Problem 41 is a reversed GP which can be transformed to standard GP. The 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 [38], [41]. Let $z(\boldsymbol{s}_I, \boldsymbol{s}_P, \rho) = \sum_{m=1}^M g_{P,m}(\boldsymbol{s}_I, \boldsymbol{s}_P, \rho)$, problem 41 is equivalent to

$$\begin{aligned}
\min_{\boldsymbol{s}_I, \boldsymbol{s}_P, \rho, \bar{\rho}, t''} \quad & \frac{1}{t''} \\
\text{s.t.} \quad & \frac{1}{2}(\boldsymbol{s}_I^H\boldsymbol{s}_I + \boldsymbol{s}_P^H\boldsymbol{s}_P) \leq P, \\
& t''\prod_m\left(\frac{g_{P,m}(\boldsymbol{s}_I, \boldsymbol{s}_P, \rho)}{\gamma_{P,m}}\right)^{-\gamma_{P,m}} \leq 1, \\
& 2^{\bar{R}}\prod_n\left(\frac{1}{\gamma_{I,n,1}}\right)^{-\gamma_{I,n,1}}\left(\frac{\bar{\rho}A_n^2 s_{I,n}^2}{\sigma_n^2\gamma_{I,n,2}}\right)^{-\gamma_{I,n,2}} \leq 1, \\
& \rho + \bar{\rho} \leq 1
\end{aligned} \tag{42}$$

where $\gamma_{I,n,1}, \gamma_{I,n,2} \geq 0$, $\gamma_{I,n,1} + \gamma_{I,n,2} = 1$, $\gamma_{P,m} \geq 0\ \forall m$, and $\sum_{m=1}^M \gamma_m = 1$. The tightness of the AM-GM inequality depends on $\{\gamma_{I,n}, \gamma_P\}$ that require successive update. At

$$\begin{aligned}
\tilde{z}(\boldsymbol{\Phi}^{(i)}) = {} & \frac{1}{2}\beta_2\rho(t_{I,0}^{(i)} + t_{P,0}^{(i)}) \\
& + \frac{3}{8}\beta_4\rho^2\left(4(t_{I,0}^{(i)})(t_{I,0}^{(i-1)}) - 2(t_{I,0}^{(i-1)})^2 + \sum_{n=-N+1}^{N-1} 2\Re\left\{t_{P,n}^{(i)}(t_{P,n}^{(i-1)})^*\right\} - t_{P,n}^{(i-1)}(t_{P,n}^{(i-1)})^*\right) \\
& + \frac{3}{2}\beta_4\rho^2\left(\frac{1}{2}(t_{I,0}^{(i)} + t_{P,0}^{(i)})(t_{I,0}^{(i-1)} + t_{P,0}^{(i-1)}) - \frac{1}{4}(t_{I,0}^{(i-1)} + t_{P,0}^{(i-1)})^2 - \frac{1}{4}(t_{I,0}^{(i)} - t_{P,0}^{(i)})^2\right)
\end{aligned} \tag{34}$$

$$\begin{aligned}
z(\boldsymbol{s}_I, \boldsymbol{s}_P, \rho) = {} & \frac{1}{2}\beta_2\rho\sum_n A_n^2(s_{I,n}^2 + s_{P,n}^2) \\
& + \frac{3}{8}\beta_4\rho^2\left(\left(\sum_n (A_n s_{I,n})(A_n s_{I,n})^*\right)^2 + \sum_{\substack{n_1,n_2,n_3,n_4 \\ n_1+n_2=n_3+n_4}} A_{n_1}A_{n_2}A_{n_3}A_{n_4}(s_{P,n_1}s_{P,n_2}s_{P,n_3}s_{P,n_4})\right) \\
& + \frac{3}{2}\beta_4\rho^2\sum_n A_n^4 s_{I,n}^2 s_{P,n}^2
\end{aligned} \tag{40}$$

iteration i, we choose [38]

$$\gamma_{I,n,1}^{(i)} = 1 \Bigg/ \left(1 + \frac{\bar{\rho}^{(i-1)} A_n^2 (s_{I,n}^{(i-1)})^2}{\sigma_n^2}\right) \tag{43}$$

$$\gamma_{I,n,2}^{(i)} = 1 - \gamma_{I,n,1}^{(i)} \tag{44}$$

$$\gamma_{P,m}^{(i)} = \frac{g_{P,m}(\boldsymbol{s}_I^{(i-1)}, \boldsymbol{s}_P^{(i-1)}, \rho^{(i-1)})}{z(\boldsymbol{s}_I^{(i-1)}, \boldsymbol{s}_P^{(i-1)}, \rho^{(i-1)})} \tag{45}$$

and then solve problem 42. The GP algorithm is summarized in Algorithm 2.

Algorithm 2 GP: Waveform and Splitting Ratio

Input $\beta_2, \beta_4, \boldsymbol{h}, P, \bar{R}, \epsilon, \sigma_n\ \forall n$
Initialize $i \leftarrow 0$, $\boldsymbol{s}_{I/P}^{(0)}$, $\rho^{(0)}$
Retrieve channel amplitude response $A_n\ \forall n$ by 3
repeat
  $i \leftarrow i + 1$
  Update GM exponents $\{\gamma_{I,n}^{(i)}, \gamma_P^{(i)}\}$ by 43 – 45
  Obtain waveform amplitude $\boldsymbol{s}_{I/P}^{(i)}$ and power splitting ratio $\rho^{(i)}$ by solving problem 42
  Compute output DC current $z^{(i)}$ by 40
until $|(z^{(i)} - z^{(i-1)})/z^{(i)}| \leq \epsilon$
Recover waveform $\boldsymbol{w}_{I/P}^{\star}$ by 36 and 38
Output $\boldsymbol{w}_{I/P}^{\star}, \rho^{\star}$

2) Semi-Definite Relaxation: In this case, waveform and splitting ratio are updated iteratively until convergence.

a) Transmit Waveform: Consider the waveform optimization subproblem. Once $\boldsymbol{\phi}$ and ρ are obtained, introduce auxiliary variables

$$t'_{I/P,n} = \boldsymbol{w}_{I/P}^H \boldsymbol{H}_n^* \boldsymbol{w}_{I/P} = \mathrm{Tr}(\boldsymbol{H}_n^* \boldsymbol{W}_{I/P}) \tag{46}$$

Therefore, 21 rewrites as

$$\begin{aligned} z(\boldsymbol{W}_I, \boldsymbol{W}_P) = &\frac{1}{2}\beta_2 \rho (t'_{I,0} + t'_{P,0}) \\ &+ \frac{3}{8}\beta_4 \rho^2 \left(2(t'_{I,0})^2 + \sum_{n=-N+1}^{N-1} t'_{P,n}(t'_{P,n})^*\right) \\ &+ \frac{3}{2}\beta_4 \rho^2 t'_{I,0} t'_{P,0} \end{aligned} \tag{47}$$

Since 47 and 30 are in the same form, we reuse 31 – 33 and bound 47 by replacing $t_{I/P,n}$ with $t'_{I/P,n}$ in 34. Hence, problem 23 is transformed to

$$\max_{\boldsymbol{W}_I, \boldsymbol{W}_P} \quad \tilde{z}(\boldsymbol{W}_I, \boldsymbol{W}_P) \tag{48a}$$

$$\text{s.t.} \quad \sum_n \log_2\left(1 + \frac{(1-\rho) W_{I,n,n} |h_n|^2}{\sigma_n^2}\right) \geq \bar{R}, \tag{48b}$$

$$\frac{1}{2}\left(\mathrm{Tr}(\boldsymbol{W}_I) + \mathrm{Tr}(\boldsymbol{W}_P)\right) \leq P, \tag{48c}$$

$$\boldsymbol{W}_{I/P} \succeq 0, \tag{48d}$$

$$\mathrm{rank}(\boldsymbol{W}_{I/P}) = 1 \tag{48e}$$

We then perform SDR and solve the optimal waveform matrix $\boldsymbol{W}_{I/P}^{\star}$ iteratively by interior-point method. $\boldsymbol{w}_I^{\star}$ and $\boldsymbol{w}_P^{\star}$ can also be extracted using randomized vectors $\boldsymbol{r}_q \in \mathbb{C}^{(L+1)\times 1}$, $q = 1, \ldots, Q$, whose entries are uniformly distributed on the unit circle $r_{q,n} = e^{j\xi}$, $\xi \sim \mathcal{U}[0, 2\pi)$. The algorithm is summarized in Algorithm 3.

Algorithm 3 SDR: Transmit Waveform

Input $\beta_2, \beta_4, \boldsymbol{h}_D, \boldsymbol{h}_I, \boldsymbol{h}_R, P, Q, \bar{R}, \epsilon, \rho, \sigma_n\ \forall n$ by 26
Initialize $i \leftarrow 0$, $\boldsymbol{W}_{I/P}^{(0)}$, $t'^{(0)}_{I/P,n}\ \forall n$ by 46
Construct $\boldsymbol{H}_n, \boldsymbol{R}_n\ \forall n$ by 26
repeat
  $i \leftarrow i + 1$
  Obtain waveform matrices $\boldsymbol{W}_{I/P}^{(i)}$ by solving problem 48
  Update auxiliary $t'^{(i)}_{I/P,n} \forall n$ by 46 for SCA
until $|(z^{(i)} - z^{(i-1)})/z^{(i)}| \leq \epsilon$
Perform EVD $\boldsymbol{W}_{I/P}^{\star} = \boldsymbol{U}_{\boldsymbol{W}_{I/P}^{\star}} \boldsymbol{\Sigma}_{\boldsymbol{W}_{I/P}^{\star}} \boldsymbol{U}_{\boldsymbol{W}_{I/P}^{\star}}^H$
Generate random vectors $\boldsymbol{r}_q\ \forall q$ with entries uniformly distributed on the unit circle
Construct candidate waveform vectors $\boldsymbol{w}_{I/P,r} = \boldsymbol{U}_{\boldsymbol{W}_{I/P}^{\star}} \boldsymbol{\Sigma}_{\boldsymbol{W}_{I/P}^{\star}}^{\frac{1}{2}} \boldsymbol{r}_q$ and matrices $\boldsymbol{W}_{I/P,q} = \boldsymbol{w}_{I/P,q} \boldsymbol{w}_{I/P,q}^H\ \forall q$
Select best solution $\boldsymbol{W}_{I/P}^{\star}$ and $\boldsymbol{w}_{I/P}^{\star}$ for problem 48
Output $\boldsymbol{w}_{I/P}^{\star}$

b) Receive Splitting Ratio Optimization: We then optimize the power splitting ratio ρ for any fixed phase shift $\boldsymbol{\phi}$ and waveform $\boldsymbol{w}_{I/P}$. In this case, the output DC current is also expressed in 47 but as a function of ρ with constant $t'_{I/P,n}$ given by 46. Since $z(\rho)$ is a monotonically increasing function of $\rho \in [0, 1]$, we replace convex objective function $z(\rho)$ with affine ρ and transform problem 23 to

$$\max_{\rho} \quad \rho \tag{49a}$$

$$\text{s.t.} \quad \sum_n \log_2\left(1 + \frac{(1-\rho)|h_n w_n|^2}{\sigma_n^2}\right) \geq \bar{R}, \tag{49b}$$

$$0 \leq \rho \leq 1 \tag{49c}$$

The optimal power splitting ratio $\rho^{\star}$ can be obtained by solving problem 49.

C. R-E Region Characterization

1) WIT Initialization: To characterize the R-E region, we initialize the algorithm to WIT mode ($\rho = 0$) and reduce the rate constraint gradually to obtain the boundary points.

a) FS-IRS: As discussed in Section III-A1, the optimal FS-IRS and composite channel are obtained in closed form. We use water-filling algorithm and matched filter to obtain optimal power allocation $p_n^{\star} = |w_{I,n}|^2$ and information waveform phase $\psi_{I,n}^{\star} = -\bar{\psi}_n$, respectively. Hence, the optimal information waveform at subband n is

$$w_{I,n}^{\star} = \sqrt{p_n^{\star}} e^{j\psi_{I,n}^{\star}} \tag{50}$$

b) FF-IRS: Consider a rate maximization problem with given information waveform $\boldsymbol{w}_I$ as

$$\max_{\boldsymbol{\Phi}} \quad \sum_n \log_2 \left(1 + \frac{|w_{I,n}|^2 \mathrm{Tr}(\boldsymbol{R}_n \boldsymbol{\Phi})}{\sigma_n^2}\right) \tag{51a}$$

$$\text{s.t.} \quad \boldsymbol{\Phi}_{l,l} = 1, \quad l = 1, \ldots, L+1, \tag{51b}$$

$$\boldsymbol{\Phi} \succeq 0, \tag{51c}$$

$$\mathrm{rank}(\boldsymbol{\Phi}) = 1 \tag{51d}$$

Problem 51 can be solved after SDR, and a best solution $\bar{\boldsymbol{\phi}}^\star$ can be obtained via Gaussian randomization method. $\boldsymbol{\phi}^\star$ can be recovered by $\phi_l^\star = \phi_l^\star / \phi_{L+1}^\star$, $l = 1, \ldots, L$. We then construct composite channel $\boldsymbol{h}$ by 4 and obtain the optimal information waveform from 50. FF-IRS and information waveform are updated iteratively until convergence. The WIT algorithm for FF-IRS is summarized in Algorithm 4.

Algorithm 4 FF-IRS: WIT Initialization

1: **Input** $\boldsymbol{h}_D, \boldsymbol{h}_I, \boldsymbol{h}_R, P, Q, \epsilon, \sigma_n$
2: **Initialize** $i \leftarrow 0$, $\boldsymbol{\phi}^{(0)}, \boldsymbol{w}_I^{(0)}$
3: Construct $\boldsymbol{R}_n$ $\forall n$ by 26
4: **repeat**
5: $\quad i \leftarrow i + 1$
6: $\quad$ Obtain IRS matrix $\boldsymbol{\Phi}^{(i)}$ by solving problem 51
7: $\quad$ Perform EVD $\boldsymbol{\Phi}^{(i)} = \boldsymbol{U}_{\boldsymbol{\Phi}^{(i)}} \boldsymbol{\Sigma}_{\boldsymbol{\Phi}^{(i)}} \boldsymbol{U}_{\boldsymbol{\Phi}^{(i)}}^H$
8: $\quad$ Generate random vectors $\boldsymbol{r}_q \sim \mathcal{CN}(\boldsymbol{0}, \boldsymbol{I}_{L+1})$ $\forall q$
9: $\quad$ Construct candidate IRS vectors $\bar{\boldsymbol{\phi}}_q = e^{j \arg\left(\boldsymbol{U}_{\boldsymbol{\Phi}^{(i)}} \boldsymbol{\Sigma}_{\boldsymbol{\Phi}^{(i)}}^{\frac{1}{2}} \boldsymbol{r}_q\right)}$ and matrices $\boldsymbol{\Phi}_q = \bar{\boldsymbol{\phi}}_q \bar{\boldsymbol{\phi}}_q^H$ $\forall q$
10: $\quad$ Select best solution $(\boldsymbol{\Phi}^{(i)})^\star$ and $(\boldsymbol{\phi}^{(i)})^\star$ for problem 51
11: $\quad$ Update composite channel $(\boldsymbol{h}^{(i)})^\star$ by 4
12: $\quad$ Obtain optimal power allocation $(p_n^{(i)})^\star$ $\forall n$ by water-filling algorithm
13: $\quad$ Obtain optimal waveform phase $(\psi_{I,n}^{(i)})^\star$ $\forall n$ by 36
14: $\quad$ Update information waveform $(\boldsymbol{w}_I^{(i)})^\star$ by 50
15: **until** $|(R^{(i)} - R^{(i-1)})/R^{(i)}| \leq \epsilon$
16: Compute phase shift by $\theta_l^\star = \arg(\phi_l^\star / \phi_{L+1}^\star)$, $l = 1, \ldots, L$
17: **Output** $\boldsymbol{w}_I^\star, \theta_l^\star$ $\forall l$

2) R-E Sample: Denote S as the number of samples in the R-E boundary.

a) FS-IRS: Since the optimal composite channel is fixed, we optimize the splitting ratio and waveform alternatively with the other being fixed. The procedure is included in Algorithm 5.

b) FF-IRS: We propose a two-layer AO algorithm to obtain the R-E region for FF-IRS-assisted SWIPT, where the inner loop updates the splitting ratio and waveform while the outer loop updates the IRS phase shifts, until convergence is achieved. The algorithm is summarized in Algorithm 6.

Algorithm 5 FS-IRS: AO Algorithm

1: **Input** $\beta_2, \beta_4, \boldsymbol{h}, P, Q, S, \epsilon, \sigma_n$ $\forall n$
2: **Initialize** $\rho_0^\star = 0$, $\boldsymbol{w}_{0,I}^\star$ by 50 and $\boldsymbol{w}_{0,P}^\star = \boldsymbol{0}$
3: **for** $s \leftarrow 1, S$ **do**
4: $\quad i \leftarrow 0$
5: $\quad$ Initialize splitting ratio and waveform by previous solution $\rho_s^{(0)} = \rho_{s-1}^\star, \boldsymbol{w}_{s,I/P}^{(0)} = \boldsymbol{w}_{s-1,I/P}^\star$
6: $\quad$ **repeat**
7: $\quad\quad i \leftarrow i + 1$
8: $\quad\quad$ Update splitting ratio $\rho_s^{(i)}$ by solving problem 49
9: $\quad\quad$ Update waveform $\boldsymbol{w}_{s,I/P}^{(i)}$ by Algorithm 3
10: $\quad$ **until** $|(z_s^{(i)} - z_s^{(i-1)})/z_s^{(i)}| \leq \epsilon$
11: $\quad$ **Return** $(R_s^\star, z_s^\star)$
12: **end for**

Algorithm 6 FF-IRS: AO Algorithm

1: **Input** $\beta_2, \beta_4, \boldsymbol{h}_D, \boldsymbol{h}_I, \boldsymbol{h}_R, P, Q, S, \epsilon, \sigma_n$ $\forall n$
2: **Initialize** $\rho_0^\star = 0$, $\boldsymbol{\phi}_0^\star, \boldsymbol{w}_{0,I}^\star$ by Algorithm 4 and $\boldsymbol{w}_{0,P}^\star = \boldsymbol{0}$
3: **for** $s \leftarrow 1, S$ **do**
4: $\quad i \leftarrow 0$
5: $\quad$ Initialize IRS, splitting ratio and waveform by previous solution $\boldsymbol{\phi}_s^{(0)} = \boldsymbol{\phi}_{s-1}^\star, \rho_s^{(0)} = \rho_{s-1}^\star, \boldsymbol{w}_{s,I/P}^{(0)} = \boldsymbol{w}_{s-1,I/P}^\star$
6: $\quad$ Initialize composite channel $\boldsymbol{h}_s^{(0)}$ by 4
7: $\quad$ *Inner loop*: Update splitting ratio $\rho_s^{(0)}$ and waveform $\boldsymbol{w}_{s,I/P}^{(0)}$ by SDR (Algorithm 5.4 – 5.10) or GP (Algorithm 2)
8: $\quad$ **repeat**
9: $\quad\quad i \leftarrow i + 1$
10: $\quad\quad$ Update IRS phase shift $\boldsymbol{\phi}_s^{(i)}$ by Algorithm 1
11: $\quad\quad$ Update composite channel $\boldsymbol{h}_s^{(i)}$ by 4
12: $\quad\quad$ *Inner loop*: Update splitting ratio $\rho_s^{(i)}$ and waveform $\boldsymbol{w}_{s,I/P}^{(i)}$ by SDR (Algorithm 5.4 – 5.10) or GP (Algorithm 2)
13: $\quad$ **until** $|(z_s^{(i)} - z_s^{(i-1)})/z_s^{(i)}| \leq \epsilon$
14: $\quad$ **Return** $(R_s^\star, z_s^\star)$
15: **end for**

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