Inverse-design of non-Hermitian potentials for on-demand asymmetric reflectivity

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Abstract: We propose a genetic algorithm-assisted inverse design approach to achieve '*on-demand*' light transport in periodic and non-periodic planar structures containing dielectric and gain-loss layers. The optimization algorithm efficiently produces non-Hermitian potentials from any arbitrarily given real (or imaginary) permittivity distribution for the desired frequency selective and broadband asymmetric reflectivity. Indeed, we show that the asymmetric response is directly related to the area occupied by the obtained permittivity distribution in the complex plane. In particular, unidirectional light reflection can be designed in such a way that it switches from left to right (or vice versa) depending on the operating frequency. Moreover, such controllable unidirectional reflectivity is realized using a stack of dielectric layers while keeping the refractive index and gain-loss within realistic values. We believe this proposal will benefit the integrated photonics with frequency selective one-way communication.

1. Introduction

The transport of light is symmetric with respect to the propagation direction in conservative, Hermitian systems, as guaranteed by reciprocity and energy conservation principles. However, unidirectional light transport devices, preventing back reflections, is highly desirable in integrated photonics to design a new generation of chip-scale optical devices for different technological applications [1–3]. As demonstrated in recent years, such breaking of wave propagation symmetry is possible in materials with complex permittivity profiles, for example, with non-Hermitian (in particular PT-symmetric) potentials. Non-Hermitian optics has attracted growing interest since reported in photonics due to several spectacular features, including unidirectional invisibility [4,5], optical switching [6], coherent perfect absorption [7,8], beam refraction [9], nonreciprocity of light propagation [10–12], nonlinear effects [13–15], and others [16]. In optics, the general requirement for PT-symmetry is that the complex permittivity, obeys the condition: $\varepsilon(r) = \varepsilon^*(-r)$ i.e., the real part of the permittivity distribution is a symmetric function and the imaginary part is an antisymmetric function in space, while this condition may be generalized to include anti-PT-symmetry or a wider class of non-Hermitian potentials [16–18], including stacked layers of purely dielectric and purely magnetic slabs [19]. In PT-symmetric potentials, the physical mechanism behind totally asymmetric light propagation is a sharp symmetry breaking-transition when a non-Hermiticity parameter exceeds a certain critical value, which is referred as exceptional point [9,10]. At such exceptional point, the eigenvalues and their corresponding eigenstates become identical that indicates a collapse of the eigenspace dimensionality. While non-Hermitian

potentials may still hold real eigenvalues in PT-phase, the eigenvalues of the systems become complex in the broken phase regime.

To date, several realizations of non-Hermitian media have been explored to exploit an asymmetric light propagating for extraordinary functionalities [20–22]. However, simple planar non-Hermitian structures comprising of a stack of dielectric layers with gain and loss are of particular interest for their compatibility with the existing fabrication technologies and availability of their theoretical models for physical insights in scattering mechanisms. The specific asymmetric behavior of non-Hermitian structures can be achieved by carefully tuning the material constituents and geometry parameters. The choice of the structural and optical parameters is usually based on intuition through trial-and-error methods. However, with the continuously increased demands for performance and integration level, such tedious trial and error methods become inefficient and time consuming in the forward design process. Therefore, solving the inverse-design problem for the desired light transport is highly desired for the development of on-demand functionalities in optical devices. Yet, no systematic study has been reported for inverse-design of non-Hermitian potentials to ensure anticipated asymmetric frequency response. So, new design approaches are essential to devise the non-Hermitian structure with given optical properties in an efficient manner. In this work, we treat the inverse-design problem as an optimization problem in which the robust optimization algorithms can be employed to accelerate the learning process of the global minimum. Generally, the optimization entails a redistribution of the ingredients of the system within the same class of the system (for instance modification of thickness of layers). However, our aim is far from being merely a blind engineering of a structure by optimization, but seeking for a more fundamental insight for the resulting structures. We start from one class of systems, in our case conservative, and require new properties of the system which are impossible to obtain in the same given class. Specifically, we require different reflections while keeping transmissions from both sides as 1. This is neither possible within the class of conservative systems nor in passively dissipative systems. Our inverse-design procedure therefore "creates" a new class of the systems, the one holding the Hilbert Transform (HT) (or Kramers Kronig relations in space), as described by Horsley et al. in a one-dimensional space [18], but also the generalized HT [23]. The heuristic optimization techniques, relying on evolutionary algorithms, such as the particle swarm optimization (PSO) [24,25] and genetic algorithm (GA) [26,27] are widely used to solve single and multi-objective problems. However, GAs are more suitable due to the ability to stochastically find the global maxima in search space for complex optimization problems without gradient information, robustness against premature convergence, ability to search the solution in parallel fashion and operate on discrete and continuous parameters simultaneously that leads to high-performance designs from integrated optical components to flat optical devices [28–32]. GA mimics the process of natural selection of the evolution and relies on three biological inspired operators: mutation, crossover and selection. A generated population (set of random solutions) evolves towards a better generation new solutions) in an iterative process to fulfil the criteria of a target (or fitness) function. Each generation is assessed based on the fitness criteria and the genes (better fitting entities) are probabilistically selected. The process reiterated until an optimal solution is found within a tolerable fitness level. For the inverse-design, the structure properties (geometry, material parameters etc) are encoded into genes and the target function to be minimized is the difference between the response produced by the configuration defined in the gene and the desired response.

To design a simple unidirectional reflectionless system, we set, as a target function, different reflectivity illuminating either from the right or from the left (in the optimum case 0% and 100%), yet the same 100% transmission both from the right and from the left. In addition, we allow the index and the *gain/loss* to vary only in particular limits. For simplicity, we take a 1D system divided into several spatial domains, with different values of the complex permittivity, expecting that the optimization algorithm brings the system to some PT-like structure [see Fig. 1]. The

idea is to seed the real part (or alternatively the imaginary part) of the complex permittivity in each section of the 1D stack and let the algorithm to choose the corresponding counterpart of permittivity for unidirectional reflection. We aim at designing periodic and non-periodic non-Hermitian structures, from a given arbitrary permittivity profile, that hold asymmetric light propagation at different spatial frequencies, as illustrated in Fig. 1(a). Figures 1(b) and 1(c) depict the asymmetric spectra corresponding to the periodic structures with discrete unidirectional reflection at two given frequencies, either in the same or opposite directions. In Fig. 1(d), we intend to design a non-periodic planar structure that exhibits broadband unidirectional propagation as it follows from the generalized HT [23]. Our work provides a feasible solution to customize multilayer non-Hermitian structures for '*on-demand*' frequency selective asymmetric response, being flexible and intrinsically different from the existing forward design methods [4,33] for tailoring the user-defined asymmetric response. Moreover, we show that the designed structures uncover the relation of the asymmetric reflectivity on the closed loop area occupied by obtained complex permittivity distribution in complex plane. The extreme asymmetric reflectivity is achieved when the closed loop area in the complex permittivity plane is maximized. In our design approach, this condition is automatically satisfied rather than being a constraint in the genetic algorithm.
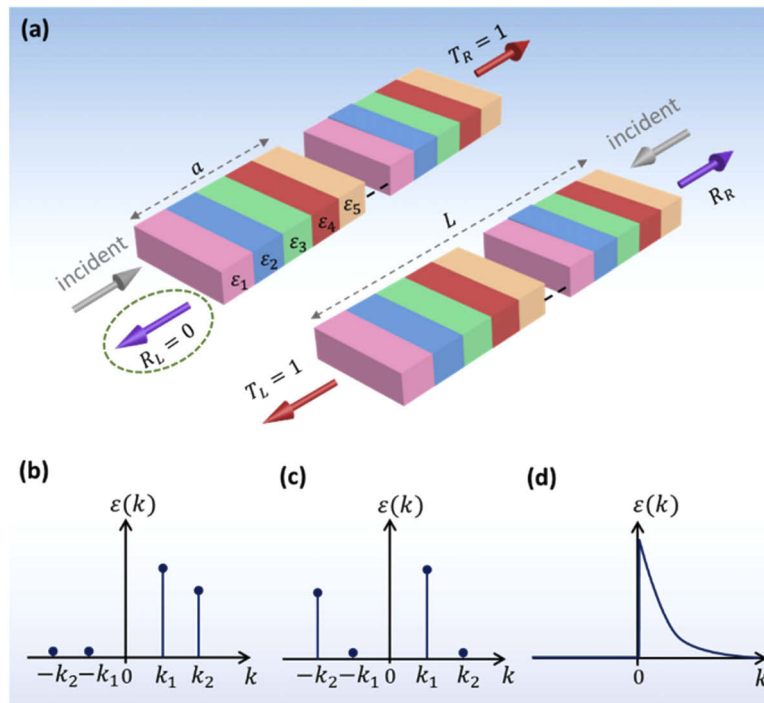

Fig. 1. Design principle for frequency selective and broadband asymmetric propagation. (a) Schematic design of a planar PT-symmetric like periodic structure for asymmetric left/right reflectance, $R_{L,R}$, and unity transmittance $T = 1$ for left/right incident waves. The length of the structure is L where each unit cell composed of five layers with periodicity, a, and complex permittivity, ε. (b,c) Asymmetric spectra of the designed permittivity distribution holding unidirectional reflection at two discrete spatial frequencies k_1 and k_2 (related to the periodicity), either in the same or opposite directions, in periodic non-Hermitian structure. (d) Non-periodic structure showing a broad-spectra unidirectional reflection.

2. Mathematical model

To realize '*on-demand*' asymmetric reflectivity, we consider an optical structure consisting of a stack of 1D layers with complex dielectric permittivity indexed as $\varepsilon^j = \varepsilon_r^j + i\varepsilon_i^j$, corresponding to the jth layer [see Fig. 1]. The structure is embedded in a homogeneous medium with uniform permittivity, ε_0. We use the TMM to obtain the scattering properties of the considered system, as the common method describing the interaction between forward and backward propagating waves in multilayered structures with coherent interfaces. The right/left propagation represents the forward/backward direction. The total field, outside the structures, may be expressed as the sum of the forward and backward propagating waves with wavevector, k, as: $E^-(z) = E_f^- e^{ikz} + E_b^- e^{-ikz}$ and $E^+(z) = E_f^+ e^{ikz} + E_b^+ e^{-ikz}$ for left ($z< -L/2$) and right ($z>L/2$) side of the structure, respectively. The continuity conditions on the different interfaces of the layered structure determine the transfer matrix, M, which couples the amplitudes of the forward and backward propagating waves at the left and right sides of the structure as follows:

$$\begin{pmatrix} E_f^+ \\ E_b^+ \end{pmatrix} = M \begin{pmatrix} E_f^- \\ E_b^- \end{pmatrix}, \quad M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \tag{1}$$

Applying the boundary conditions $E_b^+=0$ or $E_b^-=0$ for either left (L) or right (R) incident waves respectively, we obtain the transmission coefficient $t_{L,R}$, reflection coefficient $r_{L,R}$ (along with the transmittance $T_{L,R} = |t_{L,R}|^2$ and reflectance $R_{L,R} = |r_{L,R}|^2$), from the components of transfer matrix in the following form:

$$\begin{array}{ll} t_R = \frac{1}{M_{22}}, & t_L = \frac{M_{11}M_{22}-M_{12}M_{21}}{M_{22}} \\ r_R = \frac{M_{12}}{M_{22}}, & r_L = -\frac{M_{21}}{M_{22}} \end{array} \tag{2}$$

For '*on-demand*' control of the reflection properties, we need the optimal complex permittivity distribution for every given structure. For balanced gain-loss systems, the relations $\sqrt{R_L R_R} = |1 - T|$ holds from energy conservation [34], which means that when either the right or left reflection vanish then $T_R = T_L = 1$. In this article, we design structures with purposefully asymmetric and frequency dependent reflections. In particular, a genetic algorithm streamlines the design process of unidirectional reflectionless structures starting from for a given (arbitrary) real permittivity distribution. The genetic optimization searches for the optimized parameters by minimizing a predefined target function through processes which tend to mimic the process of natural evolution. The target function to be minimized, F, can be defined in different possible ways depending on the requirements. In our case, the target function is a measure of broadband unidirectionality, i.e. perfect transmission with zero reflection from one side that can be achieved with the following frequency dependent target function:

$$F(\omega) = \frac{1}{N} \int [|1 - T_R(\omega)| + |1 - T_L(\omega)| + |A(\omega)|] d\omega \tag{3}$$

where $A(\omega)$ quantifies the '*on-demand*' asymmetry in the reflectivity.

3. Asymmetric reflectivity in periodic structures

We start from a simple three-layer periodic structure with given real part of permittivity values, and search for the corresponding imaginary parts to show the frequency selective unidirectional behavior such that $A(\omega) = 2R_L(\omega)/[R_L(\omega) + R_R(\omega)]$. Then, we increase the number of layers in the system and find the optimized values for unidirectional light propagation for desired range of frequencies. The genetic algorithm efficiently optimizes the permittivity distributions for

asymmetric light effects in arbitrary layered structures. The scattering properties of optimized three, five and seven-layer systems for given real permittivity values are shown in Fig. 2. In all cases, the optimized imaginary parts permit perfect transmission from both sides while the reflection of left incident waves goes to zero, as anticipated in the target function. The spatial spectra of the optimized structure show an asymmetric coupling between wave vectors, responsible for left/right light propagation. The diminishing of spatial negative frequency components in the spectra, shown in right panels, confirms the asymmetric propagation behavior. The designed permittivity function provides left-half spatial spectrum equal to zero that is possible only when the real and imaginary parts are HT pairs. Therefore, the spatial spectrum of the designed permittivity profile serves as a guideline to decide the uniqueness of solution and target bandwidth. As the number of elements in the unit cell increases, higher wave vectors come into play and their coupling needs to be canceled to achieve the unidirectional properties. In this case, we need either larger gain/loss values or enlarged target bandwidth to cancel the coupling among the higher wave vectors, which also ensures uniqueness and a faster convergence in desired spectral range. As it is evident from the periodic nature of the proposed structure, the permittivity values form a closed loop in the complex permittivity plane. Note that the asymmetry sign and the direction of the closed loop can be changed to clockwise by reversing the sign of imaginary parts of the permittivity and equivalently allowing reflectionless behavior for right incident waves, $R_R = 0$. Precisely, such enclosed area in the complex plane of the calculated permittivity profile provides an insight of the asymmetric response of the structure, which is ultimately proportional to $(R_R - R_L)$. Note that minimum three layers are required to achieve unidirectionality in periodic structures with suitable complex permittivities such that their trajectory return to the origin, i.e forming a closed loop in complex plane.

The asymmetric response of the structure, i.e the left-right reflection asymmetry $(R_R - R_L)$, can also be analytically assessed. We start from the 1D Helmholtz equation:

$$\frac{\partial^2 E}{\partial z^2} + k^2 \varepsilon(z) E(z) = 0 \tag{4}$$

and a field composed by forward and backward waves: $E(z) = E_f e^{ikz} + E_b e^{-ikz}$. Under first Born approximation, the right to left reflection coefficient for the field amplitude is simply written as $r_R(k) = \frac{ik}{2} \int e^{2ikz} \varepsilon(z) dz$, where the integration is performed over the entire structure, and more significantly the intensity reflection coefficient can be expressed as: $R_R(k) = \frac{k^2}{4} \iint e^{2ik(z_1 - z_2)} \varepsilon(z_1) \varepsilon^*(z_2) dz_1 dz_2$. The integral can be rewritten as: $R_R(k) = \int \frac{1}{2} |\varepsilon(z_+)|^2 dz_+ \int k^2 e^{4ikz_-} dz_- + \int \frac{1}{2} (\varepsilon(z_+) d\varepsilon^*(z_+)/dz_+ - \varepsilon^*(z_+) d\varepsilon(z_+)/dz_+) dz_+ \int k^2 e^{4ikz_-} dz_-$, by applying a change of variable $z_{\pm} = (z_1 \pm z_2)/2$ and assuming that $|z_-|$ is small. Considering a periodic structure, the last expression integrated in one period can be written in the form: $R_R(k) = \left(\int \frac{1}{2} |\varepsilon(z_+)|^2 dz_+ + \int d\varepsilon_r d\varepsilon_i \right) \int k^2 e^{4ikz_-} dz_-$ where the second term inside the brackets directly involves the area enclosed in the complex plane of profile permittivity: $\varepsilon(z_+) = \varepsilon_r(z_+) + i\varepsilon_i(z_+)$ when $\varepsilon(z_+)$ is integrated along z_+ in one period. The sign of this term changes when considering the left to right reflection $R_L(k) = \left(\int \frac{1}{2} |\varepsilon(z_+)|^2 dz_+ - \int d\varepsilon_r d\varepsilon_i \right) \int k^2 e^{4ikz_-} dz_-$ and, thus, the reflection asymmetry is directly proportional to this area: $R_R(k) - R_L(k) \propto \int d\varepsilon_r d\varepsilon_i$. We note that Born approximations are valid for multilayer structures [18].

Next, we design non-Hermitian structures with unidirectional propagation directions depending on the operating frequency. As a particular example, a unidirectional reflectionless propagation in the right direction for an operating frequency ω is switched to left direction by changing the operating frequency to 2ω. We define the target function the same as in Eq. (3) but to achieve the desired frequency dependent reflectivity, $A(\omega)$, in the following form: $A(\omega) = H(\omega - \omega_0) A_L(\omega) + H(\omega - \omega_0) A_R(\omega)$ where the terms $A_L(\omega) = 2R_L(\omega)/[R_L(\omega) + R_R(\omega)]$ and $A_R(\omega) = 2R_R(\omega)/[R_L(\omega) + R_R(\omega)]$ represent the measure of asymmetry in left and right reflectivity,
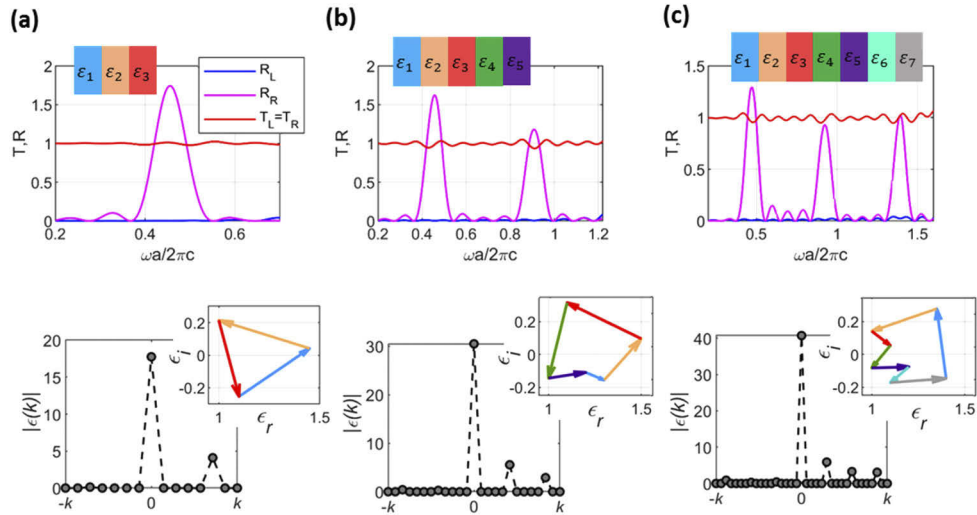
Fig. 2. Scattering properties of the optimized periodic non-Hermitian layer structure. (a) three-layer, (b) five-layer and (c) seven-layer periodic structure optimized with genetic algorithm for different real permittivity distribution seed, ε_r . (Top row) Transmittance, T, and reflectance, R, for the right and left illumination directions. (Bottom row) Spectra of the optimized complex permittivity distribution, $\varepsilon = \varepsilon_r + i\varepsilon_i$, showing the maximum asymmetry that induce unidirectional behavior. The insets illustrate the optimized complex permittivity values plotted in complex plane. Different vectors correspond to complex permittivity values in considered structures and their trajectory returns to the origin i.e forming a closed loop for unidirectionality in periodic structures. The unidirectionality occurs around frequencies corresponding to the period of the structure $\omega a/2\pi c \approx 0.45$, and at the higher harmonics of that resonant frequency. In all cases, the structure contains five periods with periodicity, a. The width of unit cell is comparable to the operating wavelength. The imaginary part of the permittivity is restricted to the range $[-0.4, 0.4]$ during optimization.

respectively. $H(\omega)$ is the step function whose value is zero (one) for normalized frequencies $\omega a/2\pi c < 0.7$ and one (zero) for $\omega a/2\pi c \geq 0.7$ to switch the unidirectional behavior from left to right (right to left) with the operating frequency, ω_0. To demonstrate such frequency dependent unidirectional effect, we consider a five layer periodic structure with given real permittivity values and determine the imaginary part of permittivity in each layer such that the system shows the right unidirectional propagation for $\omega a/2\pi c \approx 0.45$ and left unidirectional propagation for $\omega a/2\pi c \approx 0.9$ and vice versa, as depicted in Fig. 3. The asymmetry between different wave vectors in the calculated spectra clearly shows that the designed structures exhibit frequency dependent unidirectional left/right propagation.
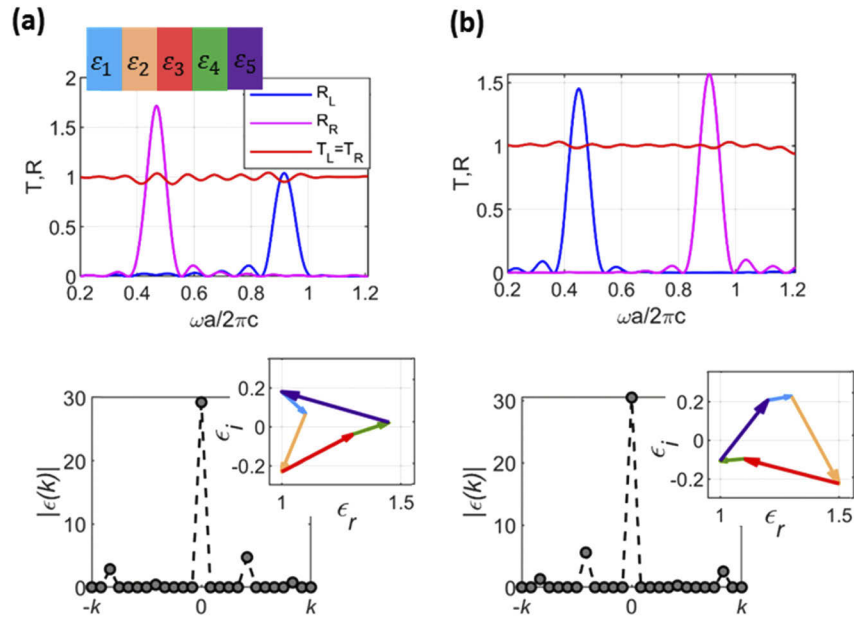
Fig. 3. Scattering properties of the optimized five-layer periodic system for frequency selective unidirectional behavior. The transmissions and reflections are obtained with genetic algorithm with different target functions and different real permittivity distribution seed. (a) right unidirectional propagation for $\omega a/2\pi c \approx 0.45$ and left unidirectional propagation for the $\omega a/2\pi c \approx 0.9$ (b) vice versa. (Top row) Transmission and reflection coefficients for the right and left illumination directions. (Bottom row) Spectra of the complex permittivity distribution for optimized structure showing the maximum asymmetry between different wave vectors that induce unidirectional behavior. The insets illustrate the optimized permittivity values, forming a closed loop, in complex plane. The imaginary part of the permittivity being restricted as in Fig. 2.

4. Asymmetric reflectivity in non-periodic structures

Finally, we design the non-Hermitian structures that showing omnidirectional reflectionless propagation for a broad range of frequencies. Such structures rely on the generalized Hilbert transform (HT) that can be implemented with sophisticated meta-atoms [35,36]. Here, we propose a simple design to realize generalized HT with planar-layered structure for arbitrary permittivity distributions. We consider a non-periodic structure in which the central layers have arbitrary real permittivity values while the lateral layers on both left and right sides contain constant real part, for instance air, as depicted in Fig. 4. The structure is modified with an appropriate choice of gain-loss regions that suppress reflection in left direction to achieve unidirectional reflectionless effect. The target function is the same as that in Eq. (3) to eliminate the reflection of the left incident waves. The results for two different real permittivity distributions are shown in Figs. 4(b) and 4(c). The determined imaginary permittivity values with genetic optimization confirm the unidirectional behavior by suppressing the reflection from the left side along with perfect transmission [see Figs. 4(a)(iii) and 4b(iii)]. The omnidirectional reflectionless behavior can be noticed in respective spectra where the spatial frequencies contributing to left propagation are eliminated [see Figs. 4(b)(iv) and 4c(iv)]. These results in setting to zero of the whole half of permittivity spectra are consistent with the generalized HT [18,23]. Therefore, the dielectric permittivities do not need any strict requirement for spatial inversion and time reversal symmetry that distinguish them from PT-symmetry. The designed non-Hermitian potentials belong to

this general class of reflectionless potentials that can be realized with locally isotropic and non-magnetic materials. Moreover, the part of our article analyses the case when a limited range of permittivity spectrum is set to zero, not the whole half-spectrum. This is more related with the generalized Hilbert transform (or could be also named generalized K.K. relation) as studied in [23]. The gain-loss profiles are designed within realistic permittivity bounds. In addition, gain-loss profile can be regularized with the iterative procedure including additional constraints to achieve the desired properties in case gain and loss values are not accessible with available materials [37]. Note that the design approach works effectively independent of number of layers in the structure for unidirectional properties. However, a large number of layers will increase the complexity of the design and will be computationally expensive. There is always a tradeoff between the resources and complexity of the structure for practical realization.
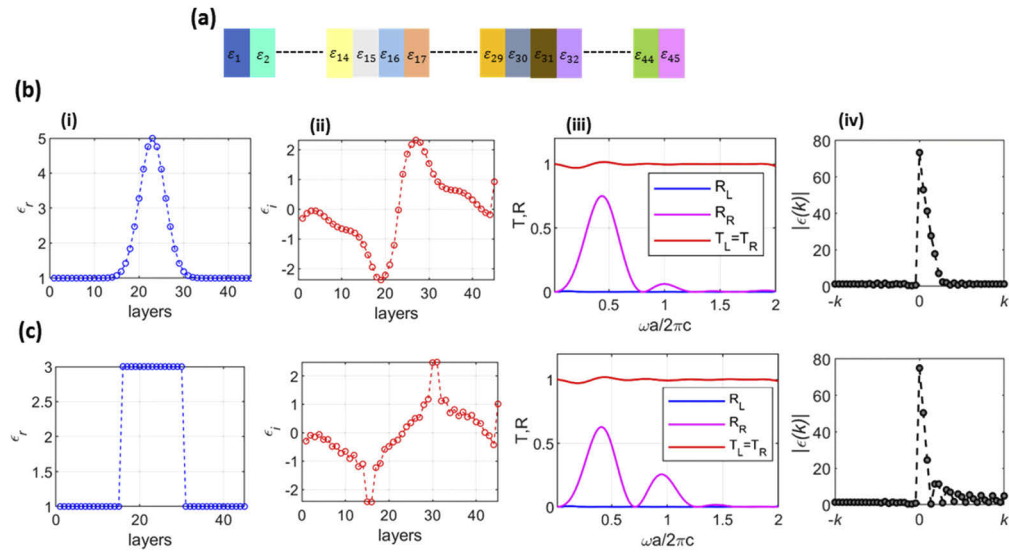

Fig. 4. Scattering properties of the designed non-periodic non-Hermitian layer structure. (a) Schematic illustration of the non-periodic structure. Two different distribution of real permittivity are considered to design unidirectional propagation for all spatial frequencies. (b) Gaussian shaped and (c) square shaped profiles of the seed. In both cases, (i) real parts of given permittivity values in each layer (ii) imaginary parts of corresponding permittivity values determined from genetic optimization (iii) transmission and reflection coefficients for unidirectional propagation (iv) Spectra of the complex permittivity distribution showing the maximum asymmetry among all spatial frequencies that allow unidirectional behavior.

5. Conclusion

We propose a systematic inverse-design approach for '*on-demand*' control of light transport by non-Hermitian systems, for the desired asymmetric spectral response. In particular, we design periodic and non-periodic non-Hermitian structures for asymmetric light propagation in a broad frequency range. We demonstrate that the genetic optimization assisted procedure allows designing frequency dependent reflectionless structures effectively for different directionalities with optimal complex permittivity distribution, and is thus a useful design tool. Such design tool explores the existence of optimal solution with anticipated properties and streamlines the inverse-design process for arbitrary permittivity distribution. The seed function with balanced effective gain and loss accelerates the convergence process. The designed structures holding the generalized HT ensure the uniqueness of the optimized solution. The resulting asymmetric behavior of

the designed structure is directly related to the enclosed area of the calculated permittivity distribution in complex space. The spectral properties confirm asymmetric reflectivity in the desired direction and frequencies ranges. Moreover, the method allows bounding permittivity within the realistic limits of actual materials. The approach can be extended to 2D and 3D systems where a large degree of freedom in space allows to optimize the permittivity distribution for different directionalities. Finally, the proposed design recipe in the optical domain can be extended to other classical wave systems, such as microwave, acoustics and elastic waves to achieve '*on-demand*' unidirectional light transport.

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