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Inverse Design of Perfectly Transmitting Eigenchannels in Scattering Media

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Light-matter interactions inside turbid medium can be controlled by tailoring the spatial distribution of energy density throughout the system. Wavefront shaping allows selective coupling of incident light to different transmission eigenchannels, producing dramatically different spatial intensity profiles. In contrast to the density of transmission eigenvalues that is dictated by the universal bimodal distribution, the spatial structures of the eigenchannels are not universal and depend on the confinement geometry of the system. Here, we develop and verify a model for the transmission eigenchannel with the corresponding eigenvalue close to unity. By projecting the original problem of two-dimensional diffusion in a homogeneous scattering medium onto a one-dimensional inhomogeneous diffusion, we obtain an analytical expression relating the intensity profile to the shape of the confining waveguide. Inverting this relationship enables the inverse design of the waveguide shape to achieve the desired energy distribution for the perfectly transmitting eigenchannel. Our approach also allows to predict the intensity profile of such channel in a disordered slab with open boundaries, pointing to the possibility of controllable delivery of light to different depths with local illumination.

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I. I. INTRODUCTION

Interference of scattered waves in random media gives rise to well-known phenomena such as enhanced backscattering, Anderson localization and universal conductance fluctuation. These phenomena are general and occur not only for electromagnetic waves, but also for acoustic, electronic and other kinds of waves^{1,2}. Recently, there has been a growing interest in another interference effect – formation of perfectly transmitting channels^{3,4}, which can greatly enhance the total transmission through opaque media⁵⁻⁸. In addition, the perfectly transmitting channels have energy density buildup deep inside the medium^{7,9-11}, opening the possibility of enhancing linear and non-linear light-matter interactions inside turbid media. Recent advances of optical wavefront shaping techniques¹²⁻¹⁷ enabled direct coupling of incident light to perfectly transmitting channels¹¹, making the depth profile of energy density dramatically different from the typical decay in a diffusive medium. To unlock the full potential of this approach for tailoring light-matter interactions in turbid media, it becomes imperative to understand what determines the spatial structure of the perfectly transmitting channels.

Recently two theoretical models have been put forward to describe the spatial profile of the perfectly transmitting channels in lossless diffusive media. Davy et al⁹ applied the supersymmetry theory to wave propagation in a quasi-one-dimensional random system and related the intensity profile to the return probability (RP) of diffusive waves. Ojambati et al^{10,18} proposed that the perfectly transmitting channel in a disordered slab is related to the fundamental mode (FM) of the one-dimensional (1D) diffusion equation. Although both models predict correctly the depth of the maximum energy density^{7,9,11,19}, they disagree quantitatively in terms of the depth profile for

the perfectly transmitting channel. So far, both models have been applied only to one-dimensional diffusion.

We have studied light transport in quasi-two-dimensional disordered systems, and showed that the spatial structure of transmission eigenchannels can be modified by the confinement geometry²⁰. For example, by adjusting the shape of the reflecting boundary of a disordered waveguide, the depth at which the energy density of a high transmission channel reaches the maximum can be moved. This enables enhancing light-matter interaction at different location inside the random medium. For many applications, inverse design is needed, namely, to design the confinement geometry to achieve the desired depth profile of energy density inside a diffusive system. This requires a prior knowledge of the relation between the geometry of the system and the spatial structure of the transmission channels. However, there is currently no theoretical model capable of establishing such relation.

In this work, we consider a two-dimensional disordered waveguide with an *arbitrary* shape, and develop a theoretical model to predict the spatial structure of the perfectly transmitting eigenchannel in the regime of diffusive transport. We further employ a projection technique, developed in physical chemistry for the particle diffusion in confined geometries²¹, to obtain an analytical relation between the depth profile of the perfectly transmitting eigenchannel and the geometry of the waveguide. With this relation, we perform the inverse design of the waveguide shape to realize the desired energy distribution for the perfectly transmitting eigenchannel. Finally, we predict the depth profile for the perfectly transmitting eigenchannel in an open slab geometry with local illumination, by simulating the lateral beam spread in a waveguide of expanding width. We find that the depth of the maximum of intensity increases with the size of the impinging beam, which provides an insight into controlling the en-

ergy distribution inside a diffusive slab with local illumination.

II. MODEL AND ITS SOLUTION

The transmission matrix, which connects the transmitted fields to the incident fields, contains the complete information about wave transport through the disordered system. Transmission eigenchannels are introduced via singular value decomposition of the transmission matrix $\hat{t} = \hat{U}\hat{\tau}^{1/2}\hat{V}^\dagger$. Here $\hat{\tau}$ is the diagonal matrix of eigenvalues of $\hat{t}^\dagger\hat{t}$ that represent the transmittance of each eigenchannel; \hat{V} is a unitary matrix that maps the incoming modes onto the eigenchannels; and \hat{U} is a unitary matrix that maps the eigenchannels onto the outgoing modes. In the regime of diffusive transport, the transmission eigenvalues have a universal bimodal distribution, independent of both the microscopical details of the disorder and the boundary shape of the system. It consists of two peaks at $\tau \sim 0$ and $\tau \sim 1$, which correspond respectively to closed and open eigenchannels^{22–25}.

Here, we consider a two-dimensional (2D) waveguide with reflecting boundaries at $y = \pm W(z)/2$. The region $0 \leq z \leq L$ is filled with lossless scattering medium characterized by the transport mean free path $\ell \ll L$. The waveguide width $W(z)$ can be either larger or smaller than the length L , corresponding to slab or quasi-1D geometry. Our aim is to predict the depth profile (cross-section averaged intensity) of the perfectly transmitting eigenchannel (PTE) with $\tau \simeq 1$, $\phi(z) \equiv W^{-1}(z) \int_{-W(z)/2}^{W(z)/2} \langle I_{PTE}(\mathbf{r}) \rangle dy$, where $I_{PTE}(\mathbf{r})$ is the intensity and $\langle \dots \rangle$ denotes the ensemble averaging. $I_{PTE}(\mathbf{r}) \equiv |E_{PTE}(\mathbf{r})|^2$, and $E_{PTE}(\mathbf{r})$ is the solution of the wave equation with the incident wave given by the eigenvector (a column vector in \hat{V}) corresponding to the eigenvalue $\tau \simeq 1$.

Diagrammatic theory was used⁹ to establish connection between the spatial profile of PTE and the diffusion return probability to the cross-section in a rectangular waveguide of constant width $W \ll L$. To determine PTE profile in the waveguides of an arbitrary cross-section and without the width constraint, we propose a phenomenological model based on the solution of the diffusion equation with the additional *ad-hoc* self-action term on the right-hand-side:

$$-\nabla_{\mathbf{r}}^2 G(\mathbf{r}; \mathbf{r}') = [1 + \alpha G(\mathbf{r}; \mathbf{r}')] \delta(z - z')/W(z), \quad (1)$$

where the diffusion coefficient D_0 is absorbed in the definition of $G(\mathbf{r}; \mathbf{r}')$. Cross-section average of its solution $\tilde{G}(z; z') \equiv W^{-2}(z) \iint G(y, z; y', z') dy dy'$ gives the normalized depth profile of PTE $\phi(z) = \tilde{G}(z; z)/\max[\tilde{G}(z; z)]$. For a rectangular waveguide in the limit of $W \ll L$ with $\alpha \equiv 0$, Eq. (1) reduces to the return probability model of Ref.⁹.

The *ad-hoc* self-action term in Eq. (1) will be justified in numerical simulations below, it is meant to account

for the effect of interference of waves that return after multiple scattering. It reflects the fact that upon the return, the coherent sum of the fields leads to the cross terms in the total intensity, similar to the weak localization correction²⁶. With the proper choice of α (to be determined below), this equation can be solved inside the disordered waveguide ($0 \leq z \leq L$, $|y| \leq W(z)/2$) with the open boundary conditions at the two ends ($z = 0, L$), $[z_0 \partial G(\mathbf{r}; \mathbf{r}')/\partial z \mp G(\mathbf{r}; \mathbf{r}')]_{z=0,L} = 0$, where $z_0 = (\pi/4)\ell$ is the 2D extrapolation length¹. The solution can be readily obtained numerically.

To obtain the analytical solution, we employ a projection technique that was developed in the study of diffusion of electrolytes in nano-pores²¹. This technique reduces the process of solving 2D diffusion equation in a complex geometry to a solution of the one-dimensional diffusion equation (along z -axis) with an effective diffusion coefficient that varies with z :

$$\mathcal{D}(z) = W(z)/[1 + (W'(z)/2)^2]^{1/3}, \quad (2)$$

where the nominator accounts for the geometrical effect of reduction of flux in a constriction, and the denominator is introduced to expand the applicability to systems with larger width variation of upto $W'(z) \simeq 1$, see Ref.²¹ for details. Eq. (1) is then transformed to yield $\tilde{G}(z; z')$ directly

$$-\frac{\partial}{\partial z} \mathcal{D}(z) \frac{\partial}{\partial z} \tilde{G}(z; z') = [1 + \alpha \tilde{G}(z; z')] \delta(z - z'), \quad (3)$$

while the boundary conditions at $z = 0, L$ remain the same. This method suits our problem because we are interested in the depth dependence of the cross-section-averaged intensity profile.

We stress that the z -dependent diffusivity $\mathcal{D}(z)$ arises from the varying width $W(z)$ in a purely diffusive waveguide where the localization corrections are negligible. In the regime where localization corrections are significant, the projection ansatz used to obtain Eq. (3) from Eq. (1) is still applicable with the effective diffusion coefficient $\mathcal{D}(z) \times D(z)/D_0$, where $D(z)$ is the cross-section averaged value of the position-dependent diffusion coefficient^{27–29} due to the localization-induced renormalization and D_0 is its unrenormalized value.

Solution of Eq. (3) can be obtained in the closed form

$$\phi(z) = \frac{(1 - \tilde{\alpha})F(z)}{[1 - \tilde{\alpha}F(z)]} \quad (4)$$

$$F(z) = \frac{4 \left(\frac{z_0}{\mathcal{D}(0)} + \int_0^z \frac{dz'}{\mathcal{D}(z')} \right) \left(\frac{z_0}{\mathcal{D}(L)} + \int_z^L \frac{dz'}{\mathcal{D}(z')} \right)}{\left(\frac{z_0}{\mathcal{D}(0)} + \frac{z_0}{\mathcal{D}(L)} + \int_0^L \frac{dz'}{\mathcal{D}(z')} \right)^2} \quad (5)$$

$$\tilde{\alpha} = \frac{\alpha}{4} \left(\frac{z_0}{\mathcal{D}(0)} + \frac{z_0}{\mathcal{D}(L)} + \int_0^L \frac{dz'}{\mathcal{D}(z')} \right).$$

$\phi(z)$ has been normalized so that $\max[\phi(z)] = 1$ and $F(z)$ is an auxiliary function, which corresponds to the

normalized solution of the same set of equations with $\alpha = 0$. The value of α (or $\tilde{\alpha}$) can be found from the waveguide with constant width.

III. VERIFICATION IN RECTANGULAR GEOMETRY

To test the analytical solution, we compare it to the numerical solution obtained by directly solving the wave equation with KWANT simulation package³⁰, see Appendix A for details. Figure 1a compares the profile of PTE computed numerically to the predictions of the two previously developed models^{9,18}. Although RP-model deviates from the numerical solution, both models agree well at $z = 0, L$. They give $\phi^{(RP)}(0) = (8/\pi) \times (\ell/L) \simeq 2.55 \times (\ell/L)$ and $\phi^{(FM)}(0) = (\pi^2/4) \times (\ell/L) \simeq 2.47 \times (\ell/L)$. The knowledge of $\phi(z)$ at one point is enough to recover the value of the coefficient $\tilde{\alpha}$. We find close values of $\tilde{\alpha} = 1 - 8/\pi^2 \simeq 0.19$ and $\tilde{\alpha} = 1 - \pi/4 \simeq 0.21$ from the two models. Below, to be specific, we use the former value. Importantly, we observe that $\tilde{\alpha}$ is a non-zero numerical constant independent of system parameters, such as the transport mean free path and the system dimension, underlining the universality of the self-action term on the right-hand-side of Eqs. (1,3). The result of Eqs. (4) is shown as dashed line in Fig. 1a, it agrees well with the result of numerical simulations. Quantitatively, the deviation (see Eq. (S1) in SI³¹) for RP-, FM-models and our Eq. (4) are 5.6%, 0.4% and 0.4% respectively. Furthermore, in Fig. 1b we verify that the same value of $\tilde{\alpha}$ applies to waveguides with varying cross-section. We stress that the agreement between numerical simulations and our model is achieved with no fitting parameters.

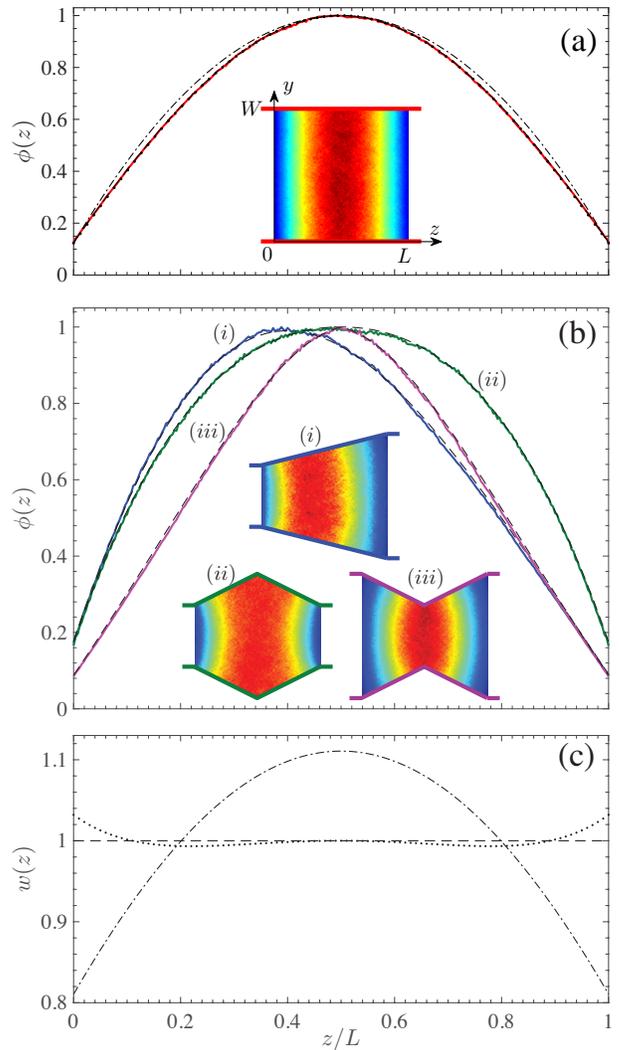


FIG. 1. (Color online) Comparison of previous models to ours in predicting the perfectly transmitting eigenchannels (PTEs) in the diffusive waveguides. (a) The cross-section integrated intensity $\phi(z)$ of the PTE in a constant width waveguide, computed numerically (bold solid line) and predicted by the RP-model (dash-dotted line), the FM-model (dotted line), and our model Eq. (4) (dashed line). The inset is 2D intensity distribution of the PTE, computed numerically, throughout this waveguide with $L/\ell = W/\ell \simeq 18.3$. (b) $\phi(z)$ for the PTEs in three waveguides of varying cross-section. Blue color: expanding waveguide, green color: lantern waveguide, purple color: bow-tie waveguide. Solid lines: numerical simulation, dashed lines: our model Eq. (4). The inset are the numerically calculated 2D intensity distribution for the PTEs in the three waveguides. The waveguide length and width at the widest point are identical to those of the waveguide shown in (a). The width at the narrowest point is equal to a half of that at the widest point. (c) The waveguide width $w_0(z)$ obtained by inverting (via Eq. (13)) the depth profile $\phi_0(z)$ predicted in the rectangle geometry by the RP-model (dash-dotted line), the FM-model (dotted line), constant width (dashed line) is shown for reference. $z_0 \ll L$ is assumed for clarity. The FM model shows less deviation from a constant width than the RP-model, but only our model produces the consistent result of constant width.

IV. IV. ARBITRARY GEOMETRY: INVERSE DESIGN

The closed-form analytical solution given in Eq. (4) establishes the relation between the shape of the diffusive waveguide and the depth profile of the PTE, thus enabling the inverse design. By introducing a normalized width function $w(z) = [W(z)/L] \times \int_0^L dz'/W(z')$, the dimensionless conductance $g = k\ell / [2 \int_0^L dz'/W(z')]$ ³², and neglecting the extrapolation length z_0 , we obtain an expression for waveguide boundary function $w_0(z)$ in terms of the depth profile $\phi_0(z)$

$$w_0(z) / \left[1 + \left(\frac{g}{k\ell} w_0'(z) \right)^2 \right]^{1/3} = \quad (6)$$

$$\left[(1 - \tilde{\alpha})(1 - \tilde{\alpha}(1 - \phi_0(z)))^3 (1 - \phi_0(z)) / \phi_0^2(z) \right]^{1/2},$$

where $k = 2\pi/\lambda$ is wave number and $\phi_0(z)$ satisfies the boundary condition $\phi_0(z = 0, L) = 0$. The extrapolation length at the boundary $z = 0, L$ can be accounted for by the following scaling

$$\phi_0(z) \rightarrow \phi(z) = \phi_0((z + z_0)/(L + 2z_0)) \quad (7)$$

$$w_0(z) \rightarrow w(z) = w_0((z + z_0)/(L + 2z_0)). \quad (8)$$

In Appendix B, we present a table of $\phi(z)$ for the waveguide geometries $w(z)$ shown in Fig. 1b.

The relation between $w(z)$ and $\phi(z)$ allows us to infer the shape of the waveguide from the depth profile of the PTE. For the depth profile of PTE predicted by the RP- and FM-models for the rectangle waveguide, c.f. Fig. 1c, we derive the corresponding waveguide shape, as shown in Figs. 1c. The shape predicted by the RP model corresponds to a waveguide with the width variation of up to 20%. In contrast, FM-model is more accurate. However, in other waveguide geometries, as shown in the SI³¹, the PTE profiles predicted by the FM-model are inconsistent with the results of the numerical simulations.

To demonstrate the power of inverse design, we change the universal profile of PTE in constant-width waveguides to a highly unusual profile of a triangle. According to Eq. (13), to have $\phi_0(z)$ increase linearly with z , we find the waveguide width $w(z) \propto \sqrt{z}$ in the leading order of $\tilde{\alpha}$. This allows us to design waveguides that support PTE with a triangular profile, as shown in Fig. 2. The waveguide boundary is described by $W(z) = W_c + \Delta W \sqrt{|z - z_c|/z_c}$, where z_c denotes the depth at which the width is the narrowest. It also closely corresponds to the maximum of the intensity profile of the PTE. The results in Fig. 2, obtained for two different values of $z_c/L = 1/2$ and $2/3$, show that it is possible to obtain waveguide geometries that have maximum concentration of energy at the desired depth.

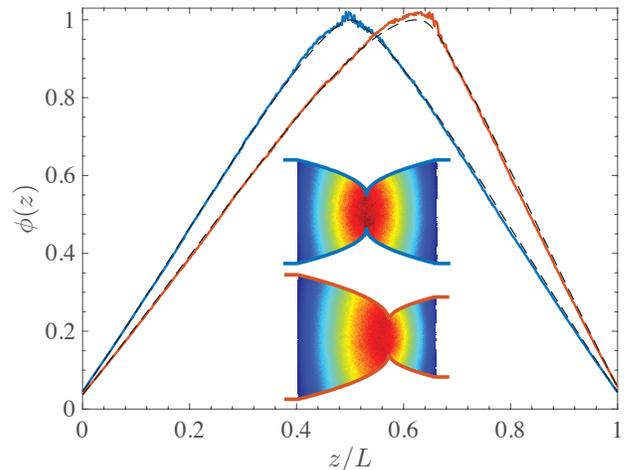


FIG. 2. (Color online) Design of waveguide shape to achieve the desired depth profile of PTE. The cross-section averaged intensity $\phi(z)$ showing an abnormal triangular dependence on the depth is obtained by the inverse design of the waveguide width $w(z)$ by Eq. (13). Bold solid lines are the result of numerical simulation, and dashed lines are the prediction by our model. The two waveguides, shown in the inset, have the PTE intensity maximum at the depth $z_c/L = 1/2$ (blue line) and $2/3$ (red line). The 2D intensity distribution of PTE are plotted in insets.

Finally, the inverse design introduced above provides an insight to controlling the depth profile of light intensity inside a *disordered slab* with local illumination. Such a geometry is common in optical experiments, and it is different from the waveguide geometry because the light will diffuse laterally as it penetrates deeper into the slab. A waveguide expanding linearly at 45° angle can be used as a proxy for studying the lateral diffusion in the slab geometry with local illumination³². In particular we consider a waveguide with expanding width $W(z) = W_1 + (W_2 - W_1) \times (z/L)$, and the tapering angle of the waveguide boundary is $\theta = \arctan[(W_2 - W_1)/2L] = 45^\circ$, to mimic the lateral diffusion in the slab. Substituting this expression into Eq. (4) leads to an important result – the profile of PTE depends on the aspect ratio of the waveguide W_1/L , see Fig. 3. It implies that in the slab geometry, the ratio between the impinging beam size and the thickness of the slab can be used to control the energy penetration. An analytical expression of the depth profile is given in Appendix B, here, we only present the formula for the depth of the maximum of the intensity

$$z_{max} \simeq L / \left[1 + \sqrt{1 + 2L/W_1} \right]. \quad (9)$$

As expected, for $W_1 \gg L$ we recover known result $z_{max} \rightarrow L/2$. As W_1/L decreases, the maximum of the energy profile is displaced towards the front surface. This result has practical applications as it offers a mechanism to scan the intensity maximum of PTE in the longitudinal direction of a disordered slab by varying the incident beam size.

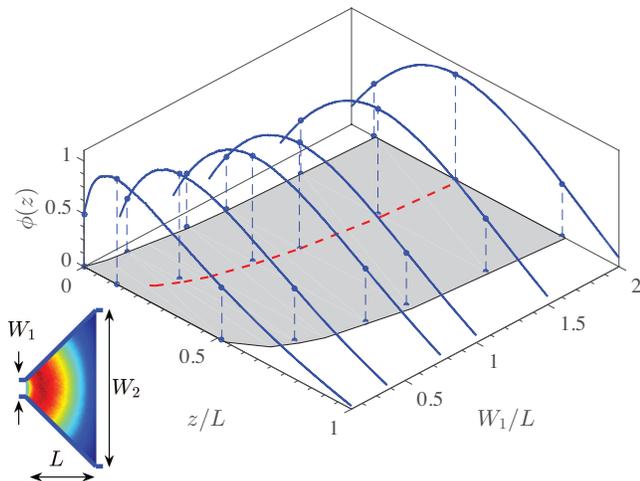


FIG. 3. (Color online) Prediction of PTE depth profile in an open slab with local illumination by approximating the lateral beam spreading with an expanding waveguide. The cross-section averaged intensity $\phi(z)$ for the linearly expanding waveguides $W(z) = W_1 + 2 \times z$ with different values of W_1 and fixed $L/\ell \simeq 18.3$. Gray area represents the region where $\phi(z)$ is greater than 1/2 of its maximum value. The position of the maximum z_{max} depends on W_1/L , which is well described by Eq. (9), bold dashed line.

V. V. CONCLUSIONS

In conclusion, we proposed a model for the perfectly transmitting eigenchannel (PTE) in the two-dimensional (2D) random system with an arbitrary shape. A self-action term was incorporated into the 2D diffusion equation for the return probability, to account for the interference effect. We employed a projection technique to reduce the 2D problem to 1D, and obtained an analytical expression relating the depth profile of the PTE to the boundary shape of the waveguide. This relation enabled the inverse design, namely, finding the waveguide shape to achieve the desired depth profile of the PTE. As an example, we predicted and verified numerically a specific shape of the waveguide in which PTE has a triangular profile. Such a profile, distinct from the universal parabolic-like profile of the PTE in the rectangle-shaped waveguide^{4,7,9,18}, yields a tighter energy distribution, that can enhance the local light-matter interaction inside the diffusive medium.

Approximating the lateral beam spreading with an expanding waveguide, we predict the depth profile for the PTE in an open slab with local illumination. The depth for the maximum intensity increases with the size of the impinging beam. Our model can be further extended to include the effect of mismatched boundary conditions³³ (via an appropriate choice of z_0), and to describe three-dimensional geometries, see Appendix C. In the latter case, the projection to one-dimension Eq. (2) shall be modified as well²¹. The results presented here are appli-

cable to electromagnetic, acoustic, electronic and other types of waves. In optics, in particular, controllable delivery of light to different depths may lead to non-invasive imaging, sensing and therapeutic applications such as e.g. 2-photon fluorescence, second harmonic generation microscopy.

VI. ACKNOWLEDGMENT

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VII. APPENDIX A: NUMERICAL SIMULATIONS

We numerically obtain the perfectly transmitting eigenchannel (PTE) by the direct solution of the wave equation using KWANT simulation package^{11,30}. It allows to conveniently compute the transmission matrix \hat{t} relating the incoming and outgoing wave amplitudes. The simulated system is a two-dimensional disordered waveguide $0 \leq z \leq L$, $|y| \leq W(z)/2$. In KWANT it is defined as a collection of coupled lattice sites in the two-dimensional rectangular grid described by a tight-binding Hamiltonian. Lack of bonds at the terminal sites at the sidewalls naturally introduces the reflecting boundary conditions. To model a passive random medium we introduce disorder by adding a random on-site potential δE_{ii} to the diagonal elements as $H_{ii} = E_0 + \delta E_{ii}$, while keeping the nearest neighbor couplings at constant value of 1. The scattering region $0 \leq z \leq L$ is connected to the leads at $z < 0$ and $z > L$ where $\delta E_{ii} = 0$. This model is well suited to describe wave scattering phenomena as long as $k\ell \gg 1$ ³⁴ where k is the wave number and ℓ is transport mean free path.

The transmission matrix \hat{t} relates the amplitudes of the propagating modes incident from the left lead ϕ_a to those of the outgoing modes in the right lead ϕ_b . Representing $t^\dagger t = \hat{V} \hat{\tau} \hat{V}^\dagger$ gives the diagonal matrix of eigenvalues τ_n and the corresponding eigenchannels V_{an} . After computing \hat{t} , we construct the input field vector $\phi_a = V_{an}$ to couple exclusively into a specific eigenchannel n . With τ_n arranged in the decreasing order, $n = 1$ corresponds to the maximum transmission eigenchannel¹¹. The parameters of the waveguides are chosen to be in the regime of a well-developed diffusive propagation $L/\ell, W/\ell \gg 1$. In this regime, the universal bimodal distribution of the eigenvalues τ_n yields the maximum at $\tau \simeq 1$. In each disorder realization we select eigenchannel with $n = 1$ and retain it only if $1 - \epsilon < \tau_{n=1} < 1$ with $\epsilon = 0.03$. Then we compute its intensity $I_{PTE}(\mathbf{r})$ and average over the ensemble of 1000

random realizations of disorder to obtain $\langle I_{PTE}(\mathbf{r}) \rangle$. $\phi(z)$ is obtained by averaging $\langle I_{PTE}(\mathbf{r}) \rangle$ over the cross-section of the waveguide.

VIII. APPENDIX B: PTE PROFILES FOR SELECT GEOMETRIES

In Sec. IV we outlined the procedure to find the depth profile of PTE $\phi(z)$ for a given shape of disordered waveguide $w(z)$, Eqs. (2,4), or other way around, to find $w(z)$ from $\phi(z)$, Eq. (13). In this appendix we present the pairs $w(z)$, $\phi(z)$ for a select group of waveguide geometries studied in this work.

1. Rectangular waveguide:

$$\begin{aligned} w(z) &\equiv 1 \\ \phi(z) &= \frac{4(1 - \tilde{\alpha})\zeta(1 - \zeta)}{1 - 4\tilde{\alpha}\zeta(1 - \zeta)} \\ \zeta &= (z + z_0)/(L + 2z_0). \end{aligned}$$

2. Linearly expanding waveguide:

$$\begin{aligned} w(z) &= \left(\frac{W_1}{W_2 - W_1} + \frac{z}{L} \right) \log \frac{W_2}{W_1} \\ \phi(z) &= \frac{4(1 - \tilde{\alpha})\zeta(1 - \zeta)}{1 - 4\tilde{\alpha}\zeta(1 - \zeta)} \\ \zeta &= \frac{\frac{z_0}{W_1} + \frac{L}{W_2 - W_1} \log \frac{w(z)}{w(0)}}{\frac{z_0}{W_1} + \frac{z_0}{W_2} + \frac{L}{W_2 - W_1} \log \frac{w(L)}{w(0)}}. \end{aligned}$$

Here $W_{1,2}$ denote the widths at $z = 0, L$.

3. Bowtie/lantern waveguide:

$$\begin{aligned} w(z) &= \left(\frac{W_2}{W_1 - W_2} + \left| 2\frac{z}{L} - 1 \right| \right) \log \frac{W_1}{W_2} \\ \phi(z) &= \frac{4(1 - \tilde{\alpha})\zeta(1 - \zeta)}{1 - 4\tilde{\alpha}\zeta(1 - \zeta)} \\ \zeta &= \frac{\frac{z_0}{W_1} + \frac{L/2}{W_2 - W_1} \log \frac{w(z)}{w(0)}}{\frac{z_0}{W_1} + \frac{z_0}{W_2} + \frac{L}{W_2 - W_1} \log \frac{w(L)}{w(0)}}. \end{aligned}$$

Here W_1 denote the widths at $z = 0, L$, and W_2 is the width at the mid-point $z = L/2$ of the waveguide.

IX. APPENDIX C: GENERALIZATION TO 3D

In this Appendix we generalize our model Eqs. (1,2,3) to three-dimensional systems. We consider axially sym-

metric waveguide of diameter $W(z)$ where z is the axial coordinate. This corresponds to cross-section $A(z) = \pi W^2(z)/4$ which varies longitudinally. 3D version of Eq. (1) with a planar source at z' now reads

$$-\nabla_{\mathbf{r}}^2 G(\mathbf{r}; \mathbf{r}') = \left[1 + \alpha^{(3D)} G(\mathbf{r}; \mathbf{r}') \right] \delta(z - z')/A(z), \quad (10)$$

where as in Eq. (1) the diffusion coefficient has been absorbed in the definition of $G(\mathbf{r}; \mathbf{r}')$. Open boundary conditions are to be applied at the two ends ($z = 0, L$), $\left[z_0^{(3D)} \partial G(\mathbf{r}; \mathbf{r}') / \partial z \mp G(\mathbf{r}; \mathbf{r}') \right]_{z=0,L} = 0$, where $z_0^{(3D)} = (2/3)\ell$ is the 3D extrapolation length. Projection from the 3D waveguide geometry to 1D system with spatially-varying diffusion coefficient can be accomplished analogously²¹ to 2D case (compare to Eq. (2)), with

$$\mathcal{D}^{(3D)}(z) = A(z) / \left[1 + (W'(z)/2)^2 \right]^{1/2}, \quad (11)$$

Eq. (10) is then transformed to yield $\tilde{G}(z; z') \equiv A^{-2}(z) \int \int G(\mathbf{r}; \mathbf{r}') dx dy dx' dy'$ directly

$$-\frac{\partial}{\partial z} \mathcal{D}^{(3D)}(z) \frac{\partial}{\partial z} \tilde{G}(z; z') = \left[1 + \alpha^{(3D)} \tilde{G}(z; z') \right] \delta(z - z'), \quad (12)$$

while the boundary conditions at $z = 0, L$ remain the same as for Eq. (10).

The normalized depth profile of PTE $\phi(z) = \tilde{G}(z; z) / \max[\tilde{G}(z; z)]$ can be found in the analytical form of Eqs. (4,5) with substitution of $\mathcal{D}(z) \rightarrow \mathcal{D}^{(3D)}(z)$ and $\tilde{\alpha} \rightarrow \tilde{\alpha}^{(3D)}$. The former is given by Eq. (11). The value of the constant $\tilde{\alpha}^{(3D)}$ can be established using the same procedure as in Sec. III – comparing the result to the waveguide with $W(z) = \text{const} \ll L$ in RP- or FM-model. We find $\tilde{\alpha}^{(3D)} = 1 - 3/\pi \simeq 0.045$ and $1 - 3\pi^2/32 \simeq 0.075$ respectively.

Inversion of the solution can be made similar to Eqs. (13,7,8). Introducing a normalized area function $a(z) = [A(z)/L] \times \int_0^L dz'/A(z')$, and neglecting the extrapolation length z_0 , we obtain an expression for waveguide boundary function $a_0(z)$ in terms of the depth profile $\phi_0(z)$

$$a_0(z) / \left[1 + (W'_0(z)/2)^2 \right]^{1/2} = \quad (13)$$

$$\left[(1 - \tilde{\alpha})(1 - \tilde{\alpha}(1 - \phi_0(z)))^3 (1 - \phi_0(z)) / \phi_0'^2(z) \right]^{1/2},$$

where subscript zero refers to $z_0 \rightarrow 0$ approximation, which is relaxed using scaling procedure in Eqs. (13,8).

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