

Ollscoil na hÉireann, Corcaigh
National University of Ireland, Cork



**Modelling Wave Transport in Random Media
for Wavefront Shaping Applications**

Thesis presented by

Michael Raju

for the degree of

Doctor of Philosophy

University College Cork

Department of Physics

Head of Department: Prof. John McNerney

Supervisor: Prof. Stefan Andersson-Engels

Co-supervisor: Prof. Eoin O'Reilly

2022

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Declaration

This is to certify that the work I am submitting is my own and has not been submitted for another degree, either at University College Cork or elsewhere. All external references and sources are clearly acknowledged and identified within the contents. I have read and understood the regulations of University College Cork concerning plagiarism and intellectual property.

Michael Raju

Abstract

The central theme of my thesis is to develop various analytical and numerical methods, for the coherent control of waves to assist various wavefront shaping applications in random disordered media. This resulted in the development of 2D scalar wave transport modelling frameworks, analytically and computationally, from the scratch. The modelling frameworks cover both frequency domain and time domain. In the frequency domain, the generalised scattering matrix (S matrix) incorporating evanescent modes is used to study the transport properties. The wavefront shaping methods in the frequency domain involve eigenchannels and iterative phase conjugation for the enhancement of total transmission through slab disorders and disordered constrictions. The generalisation of the conventional Fisher-Lee relations to incorporate evanescent modes is presented in the thesis. S matrices of spatially correlated disorders are estimated using the generalised Fisher-Lee relations, incorporating the Green's function perturbation method. The comparison between the conventional diffusion theory and the wave transport theory is presented, which involves the cascading of S matrices and the transmission scaling law. The relationship between the spatial correlation of the disorder and various transport properties are also investigated in this comparison. In the time domain, using the finite difference time domain scheme, wavefront shaping involving iterative phase conjugation onto a space-time modulated (STM) guide-star region operating in the Raman-Nath regime, is investigated. The intention of studying the STM is to investigate the potential of the acousto-optic effect for imaging through random media. In the time domain, the effect of sample decorrelation due to Brownian motion on the stability of the focussing is also studied using the Langevin equation. The discussion of the analytical and numerical aspects of the developed models, along with the availability of simulation codes written in Matlab, may be of interest to wavefront shaping researchers interested in characterisation of various wave transport behaviours.

Acknowledgement

I am deeply thankful to many.

Foremost, I would like to thank Prof. Stefan Andersson-Engels, for his scientific visions and the unwavering academic guidance, which were crucial for the development of contents of this thesis. Stefan, about whom the phrase ‘the vitality of the youth with the wisdom of the age’ could be confidently said, was always available and approachable in person, to discuss and learn from. I would also extend my sincere gratitude to Stefan, for giving me the academic freedom to pursue the means to achieve the intended research goals, which helped me to study about the topics presented in the thesis in good spirits. His enthusiasm to maintain a great team spirit and his scientific inquisitiveness in organising various brainstorming sessions, have helped me to sustain my morale during the PhD years. Stefan, always being calm and composed and in great physical fitness, has influenced me to understand the importance of emotional and physical health, especially to endure the PhD life. His high priorities regarding the holistic well-being of his team, will stay with me forever as a lifelong takeaway. His willingness to patiently listen and learn from others with great inquisitiveness, is a humbling experience for me to watch and learn from him.

I would like to thank the Science Foundation of Ireland (*SFI*), for funding my PhD studies through the *SFI* research professorship awarded to Stefan, titled ‘Novel applications and techniques for in vivo optical imaging and spectroscopy’ (*SFI/15/RP/2828*). Such a grant lead Stefan to relocate from Lund, Sweden to Cork, Ireland in 2016, to set up his new team (*Biophotonics@tyndall*) from scratch. I was fortunate in joining the team in 2017 as an early member and to see the team build up in size, from three members to around forty as of now. It is a great feeling to see our *Biophotonics@Tyndall*, being a center of excellence in the field of biophotonics in Ireland under the leadership of Stefan. I’m thankful for being in such an eco-system which supports the holistic growth of the doctoral students in the field of biophotonics.

This thesis couldn’t have been formulated without the love and support from my wife, Mrs. Diana Joseph. She was a lecturer in India and relocated herself from India to Cork, for joining me to live together even though she couldn’t work in Ireland due to visa restrictions (being dependent on a student visa holder). I am deeply indebted to Diana and would like to dedicate this thesis to her, for being selfless in wholeheartedly supporting me, with her never-ending love and optimism. I’m fortunate to have her long-standing companionship in our journey together, since our school days.

I’m lucky to have great post-doctoral teammates, Dr Baptiste Jayet and Dr Jacqueline Gunther. Thank you Baptiste, for our weekly personal discussions for brainstorming and

exploration of various aspects of the research with your never-ending enthusiasm and motivation. Also, I would like to thank Baptiste and Jakie for their review comments and suggestions which helped me to improve my writing and thinking process. I extend my gratitude towards the graduate supervision committee members, Prof. Eoin O'Reilly (co-supervisor) and Prof. Frank Peters (Monitor), for their guidance, suggestions and constructive comments. I would like to thank Prof. Mats Gustafsson, Lund University, for all the discussions we had. Many thanks to my fellow PhD scholars Michael Amis, Marcelo, Andrea, Siddra, Gokhan, Lorenzo and Jean, for all the good times we had in the team. Thank you Cerine, Haiyang, Shree and Eduardo for all your valuable suggestions, help and motivation. Many thanks to Sarah Donovan for helping me through various administrative processes in Tyndall and UCC.

Living in Cork city, Ireland, as a single-income couple dependent solely on the PhD stipend, was possible because of the immense support from our landlords Mr. Gerry O'Shaughnessy and Dr. Ben O'Shaughnessy. Thank you very much for providing us an opportunity for sustainable living in Cork and literally a home away from home. It was a great pleasure to have you Aoife, Seth, Andres, Clare, Ferga and other Knocknacool-ians, as our lovely housemates.

Thanks to the organisers of the French 'GdR complexe' workshops and summer schools, which provided great opportunities to learn about the fundamental aspects of the wave transport in complex media. The summer schools and workshops hosted in Corsica and Paris were really helpful in understanding the concepts and to interact with many other researchers in the field. Special thanks to Prof. Chia Wei Hsu (University of Southern California), for giving me an introduction to the modelling of transmission matrices during the Corsica summer school, 2018.

Thanks to Prof. Jacopo Bertolotti's (University of Exeter) #PhysicsFactlet tweets. The visualisations of various concepts in physics contained in those tweets were always helpful in clarifying fundamental ideas regarding wave scattering and transport. Youtube lectures of Prof. V Balakrishnan (NPTEL, IIT-Madras) and Prof. Raymond C. Rumpf (University of Texas at El Paso) were immensely helpful in understanding some of the core ideas needed for the modelling. Many thanks to Prof. N. Sujatha, IIT-Madras, my master's thesis supervisor for introducing me to the amazing world of transport theory in random media.

L^AT_EX using the KOMA-Script and the kaobook class was used to typeset this thesis. The source code used for typesetting was obtained from :<https://github.com/fmarotta/kaobook> and thanks to the developers behind.

I would like to thank all the people who directly or indirectly helped me to completely stay away from a possible COVID-19 infection during the final two years of my PhD studies. Finally, thanks to my parents, parents-in-law and siblings, for all the support they gave me to pursue an academic life.

Three rules of research (in modelling)

1. If a first-principle solution is available, then don't use an approximation.
2. If you have to use an approximation, then make sure it is analytical.
3. If an analytical approximation is not available, then switch to another research problem.
4. (If one has act professional, by not switching the given problem, then) I'm not listening to rules 1-3.

Dr Michael I. Mishchenko,
Maniac Talk, January 26, 2015,
"How much first-principle physics
do we need in remote-sensing
and atmospheric-radiation research."

Preface

The coherent control of waves in disordered medium through wavefront shaping has been an actively researched topic in various physical domains such as acoustics and electromagnetics. The experimental coherent control for focussing light outside a disordered medium[1], for enhancing total light transmission through a disorder[2, 3] and inside[4] a region enclosed by disorder have been reported. Preferential deposition[5–7] of energy inside a disorder has also been a potential application within the scope of the coherent control of light. Access to the interferometric phase measurement systems and wave shaping devices such as spatial light modulators have helped to accelerate the research on coherent control experiments using light, especially using optical[8] or acousto-optical[4] transmission matrices since the 2010s. On the other hand, the analytical aspects associated with the theory of coherent wave transport have been in active research since the 1980s, having roots from the scalar wave perturbation theory[9, 10] and the random matrix theory[11, 12]. Theoretical developments which were initially used to address various aspects of quantum transport, eventually got adapted into the realm of classical waves since the 1990s. Phenomenon such as long-range correlation[13, 14] of multiply scattered waves well researched through the 1990s, has been proved to play significant roles in total transmission enhancement[2, 3, 15] and focussing contrast[16] associated with wavefront shaping experiments in the 2010s. For better insights regarding these coherent transport aspects, modelling of the scattering matrices (S matrices) and the wave field visualization of the associated transport phenomena would be particularly helpful. The analytical and numerical implementation of such simulation models used in the context of wavefront shaping, is the central theme of this thesis.

Researchers coming from different fields who are new to the field of wave transport through random media for wavefront shaping applications, usually would need to do a literature review spanning the mesoscopic wave transport theory. It involves the perturbation theory and the random matrix theory in the quantum or the classical contexts. Publications such as [17–19] makes the aspects of mesoscopic wave transport theory accessible to researchers from other domains. It is in this context that the thesis is placed so that researchers new to the modelling of wavefront shaping, who are familiar with the classical wave scattering theory, can leverage from the thesis without spending much time for learning the coherent mesoscopic quantum transport theory. All the analytical and computational modelling done for the thesis was done from scratch by me in MATLAB, with an intention to be eventually published as open source code package with the *GNU* General Public License. These studies involve both frequency domain and time domain, addressing the 2D scalar Helmholtz wave equation without any absorption or gain. The scalar Helmholtz wave equation was used mainly to maintain the generality of

the applications for a diverse range of physical domains. In addition to that, the transport analysis was done as a $2D$ problem mainly for the computational easiness. Although the analytical derivations presented addresses only the $2D$ scalar transport, the concepts can be generalised to $3D$ without much difficulty due to the involvement of frequency domain Green's function, boundary integrals and the finite difference time domain methods. All the computational modelling and the associated results presented in the thesis were implemented using a desktop PC with a modest configuration of 64 GB of RAM, an AMD Ryzen 7 2700X (eight-core, 16 CPU, 3.7GHz) processor and a NVIDIA GeForce GTX 1050 Ti GPU. The time domain methods were accelerated using the GPU in Matlab and the frequency domain methods were implemented only using the CPU due to the larger memory requirement associated with the Green's function methods. For the analytic derivations presented in the thesis, Mathematica was used for the symbolic computation of various expressions.

The modelling studies done in the frequency domain were about the numerical estimation of the generalised scattering matrix (S matrix) containing both propagating and evanescent modes. In the first chapter, the generalized S matrix proposed by Carminati et al.[20] was numerically estimated by generalizing the conventional Fisher-Lee relations[21], based on the $2D$ scalar wave equation. These evanescent modes are particularly significant in the sub-wavelength focussing applications involving near-field scanning optical microscopy probes[22]. The relationship between the Kirchhoff-Helmholtz boundary integral formulation and the conventional Fisher-Lee relations was given by[23] in the context of quantum particle scattering. Such a conventional relation is generalised in this thesis to obtain the Fisher-Lee relations involving the evanescent modes. For implementing the Fisher-Lee relations, the Dyson's Green's function perturbation method is used, which is usually a memory intensive process. An attempt to save memory is implemented by iteratively solving the scattering problem, by taking slices of scatterers in the each iteration step. The modelled S matrices satisfy the extended or the generalized unitarity and reciprocity relations proposed in[20, 24] as well. The S matrix contains the transmission matrices of the disorder with the wave incidence from both the left side and the right side. The propagating part of the transmission matrix is used to visualise and estimate transmission eigenchannels from both left side and right side with enhanced transmission. These transmission matrices are also used for iteratively phase conjugating the waves from both sides of the disorder for focussing applications. The S matrices of thinner slabs are cascaded to create thicker slabs using the S matrix cascading rule. Such a cascading method helps in easy generation of ensembles of S matrices by randomly shuffling the order of cascading. Spatially correlated disorders were used for estimating the S matrices. This is because the spatial correlation of scatterers is common among biological tissue samples[25]. The spatial correlation also helps to tailor the transport properties such as the scattering mean free path (l), the transport mean-free path (l^*) and the anisotropy of the disorder as demonstrated in chapter 2. The two parameter scaling of total transmission with respect to various transport properties are also discussed. Such a

scaling law implies that one may not always need to model large samples with millions of scatterers to understand the transport physics. Instead, one could model smaller samples and express the transport in terms of L/l^* where L is the longitudinal thickness of the sample in a flux conserved scattering system.

The frequency domain methods presented in the thesis have the general advantage being analytically tractable to a certain extent. Although the contents of the thesis is only about steady state wave transport, some of the interesting topics to be researched was tough (although not impossible) to be implemented in the frequency domain. Hence, the finite difference time domain (*FDTD*) methods were also studied to address some of the time dependent phenomena such as the disorder decorrelation due to the Brownian motion during single speckle focussing and the space-time modulation (*STM*) (an example being the acousto-optic effect).

Wavefront shaping in general is always in competition against the random motion inside the disordered sample, leading to the scrambling of the shaped wavefront. Therefore a quantitative study on the effect of the Brownian motion on single speckle focussing through phase conjugation, is presented in chapter 3. Such a study involves the Langevin equation of motion for the Brownian scatterers. An *FDTD* method to simulate the Langevin dynamics, is used together with the wave transport *FDTD* method to simulate the effect of the Brownian motion.

The *STM* region surrounded by the disorder could be used as a “guide-star”[26–28] to focus light inside random media. Inspired from various experiments[4, 29], the iterative phase conjugation through a *STM* region is modelled in chapter 4 to focus light inside a disordered region. This is to demonstrate the breaking of the acoustic diffraction limit in the conventional acousto-optic imaging. In addition to that, various aspects regarding the *STM* diffraction are also reviewed in chapter 3 to demonstrate the two regimes of operation, namely the Bragg regime and the Raman-Nath regime. It needs to be emphasised that the exact modelling of the acousto-optic effect in the time-domain, could be challenging due to the huge difference in the temporal frequency of light and sound waves. This would naturally lead to the need for a large number of time-stepping in the *FDTD* scheme. Hence the term *STM* is used in this thesis, where the temporal frequency of the modulation (ω_{mod}) is very high compared to that sound waves. As an example, in this chapter ω_{mod} is a fraction of the light temporal frequency (ω_0) such that $\omega_{mod}/\omega_0 = 0.2$. As *STM* is a generalisation to the acousto-optic effect, the basic transport physics remain the same. Therefore, the term acousto-optics is purposefully avoided in this thesis and instead the term space-time modulation is used. The relation between eigenchannels (shown in chapter 1) with that of the iterative phase conjugation method, is validated in chapter 4 using a disordered constriction.

Much care is given to develop and validate models to ensure the flux conservation such that the transmission and reflection adds to unity. This is because the physics of the problem and the scalability of the models with respect to the size, can be explained in terms

of flux conservation principles involved. There are no arbitrary or free parameters (which cannot be analytically tracked to a first principle equation) defined in the thesis. Hence, all the terms used in the thesis, derives their existence from the fundamental principles involved. To ensure the flux conservation easily by estimating the transmission and reflection at only two surfaces, reflecting (mirror) boundary conditions are implemented at the transverse boundaries for both the frequency domain and the time domain wave transport models. One could also use the periodic boundary condition with ease in the frequency domain instead of the reflecting boundary condition, but such a periodic boundary condition becomes cumbersome in the time domain models. Therefore, for a unified outlook on both the frequency domain and time domain, the same transverse reflecting boundary condition is implemented. For comparing the results and trends in this thesis against an experiment, the assumption of flux conservation has to be strongly held. This is because the wave modelling of the samples of similar size used in the experiments are prohibitively harder to implement due to the limited computational capacity one has.

These methods presented in the thesis may be of interest to the wavefront shaping researchers to explore the modelling aspects of the associated transport theory.

The methods in Frequency Domain for wavefront shaping

1

1.1 Introduction

The main objective of this chapter is to discuss in detail, the analytical formulations and the numerical implementations, involved with the frequency domain modelling of the wave transport phenomena in 2D random media, for wavefront shaping applications. The scope of this study with respect to the transport phenomena, is within the ballistic and the diffusion regimes. The central theme of this chapter is the computational estimation of the generalised[20, 24] scattering matrix (S matrix), involving both propagating and evanescent wave modes associated with the wave scattering problem, through non-absorbing random media. Using such a generalized S matrix for studying the wave transport problem, is particularly advantageous due to the following reasons. 1) The generalised S matrix, completely characterises the wave scattering response of any arbitrary wave, incident on the random slab. Therefore, one could use the information contained in the S matrix, to directly estimate an incident wave state, which yields the desired transport behaviour through the medium. 2) It is possible to cascade several S matrices associated with thinner slabs, to obtain the total effective S matrix of the thicker slab formed by cascading of the thinner slabs.¹ 3) The flux conservation and the reciprocity properties of the transport phenomena, cause the S matrix to have the generalised unitarity and reciprocity properties, which can be used as a benchmark to test the accuracy and the correctness of the developed coding framework. 4) The random S matrix (which is covered under the theory of random matrices) provides us an abstraction layer encapsulating the macroscopic transport behaviour, without being concerned much about the finer (microscopic) details of the scatterer configuration. The first half of the chapter explains the methods used to estimate the generalised S matrix for the quasi-1D transport problem. This is followed by the extension of the methods to account for the 2D transport problem, incorporating the transverse diffusion within the slab. Before we get into the estimation of the generalised S matrix containing evanescent modes, several concepts have to be discussed and the best place to start is at the nature of wave equation used for modelling.

The wave transport phenomena in random media, observed in various domains of physics such as quantum, electromagnetic, acoustic and seismic physics, share very similar properties with respect to their transport behaviour. This could possibly be due to the similar mathematical form of the governing wave equations² and the ability to use various statistically averaged transport parameters, such as the scattering (l) and transport mean free (l^*) paths, to address wave transport across many different fields of physics. To maintain the generality of the wave transport modelling across various physical domains, this thesis adopts the use of the scalar Helmholtz wave equation[18] as the governing equation

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[20]: Carminati et al. (2000), 'Reciprocity, unitarity, and time-reversal symmetry of the S matrix of fields containing evanescent components'

[24]: Byrnes et al. (2021), 'Symmetry constraints for vector scattering and transfer matrices containing evanescent components: Energy conservation, reciprocity, and time reversal'

1: The cascading of S matrices relaxes the computational memory requirement to solve a large scattering problem, by solving the problem piecewise.

2: Refer to section II of [18] or 2.1 of [17] for details regarding the similarity between wave equations in different physical domains such as electronics and optics.

[18]: Rotter et al. (2017), 'Light fields in complex media: Mesoscopic scattering meets wave control'

[17]: Akkermans et al. (2007), *Mesoscopic physics of electrons and photons*

for exploring the mesoscopic^[17] transport phenomena. Also, the wave scattering problem presented in the thesis, is analysed as a 2D transport problem instead of analysing it in 3D, mainly to get around the need for large computational power to estimate the S matrices in 3D. The scalar Helmholtz wave equation^[18] in the temporal frequency domain is given as

Scalar Helmholtz wave equation

$$[\nabla^2 + k_0^2 \mu_r \tilde{\epsilon}_r(r)] \tilde{E}(r) = 0, \quad (1.1)$$

where $\tilde{E}(r)$ denotes the complex valued³ scalar wave field as a function of the position $r = (z, y)$, $k_0 = 2\pi/\lambda_0$ is the free space wave vector magnitude, λ_0 the free-space wavelength, $\tilde{\epsilon}_r(r)$ the relative dielectric permittivity constant forming the scattering strength of the random media and μ_r , the relative permeability constant which is usually taken as unity for a non-magnetic medium. As $\tilde{E}(r)$ corresponds to the complex field value at a certain position, the time harmonic dependence⁴ can be explicitly brought in as $\tilde{E}(r, \omega) = \tilde{E}(r)e^{-i\omega t}$ where ω is the temporal frequency and t the time. In the 2D electromagnetic wave scattering problems, the Maxwell's equations for the $\tilde{E}$ field (polarised perpendicular to plane of incidence) simplifies⁵ to the scalar Helmholtz equation (given in equation 1.1). This reduces the computational complexity in 2D compared to the vector wave equation related to the electromagnetic wave transport in 3D.⁶ Hence, it is safe to address the 2D electromagnetic wave transport problem using the scalar Helmholtz equation, still covering rich physics in regards to the transport phenomena.

Given a partial differential equation such as the wave equation, the main objective in the next sections would be to solve this equation to uniquely estimate the total field $\tilde{E}(r)$ for a given scattering medium characterised by $\epsilon_r(r)$ and a given incident wave, by specifying the desired boundary condition. For formulating the solution to such a problem in the frequency domain, the concept of Green's function will be extensively used in this chapter. The Green's function in the random medium, together with the Kirchhoff-Helmholtz boundary integral formulation of the wave equation, will be used to uniquely solve the wave scattering problem in the following sections. Eventually, such a boundary integral formulation will be used to visualise the total field inside the disordered region and also to estimate the generalised S matrix containing the evanescent modes. The overview of the contents for this chapter, is given in Figure 1.1. The logical flow of the description of the theory (as given in the flowchart) is contained in this chapter and any digression to this main logical flow, is provided in the appendix. These digressions are mainly the derivations to be served as proofs for the assertions made in the chapter. Such an appendix would be useful for pedagogical purposes and also for the completeness of the thesis. As per the flowchart, first, the geometry of the modelling region and the associated eigenmodes satisfying the boundary conditions of this geometry, are explained. The chapter starts by exploring the quasi-1D transport problem. Towards the end of the chapter, the conventionally addressed quasi-1D problem is modified to the 2D transport problem, incorporating a finite sized

3: The tilde symbol $\sim$ over E implies that the field is analysed in the frequency domain and can be complex valued. In the Chapter 3, the $\sim$ symbol is dropped as the E field is real in the time-domain models.

4: Usually in physics and particularly in this thesis, the time harmonic dependence is taken as $e^{-i\omega t}$ where i is the imaginary number. On the other hand, in some of the engineering disciplines, the sign convention used for the harmonic dependence is $e^{+i\omega t}$.

5: The analytical proof for the statement that the Maxwell's equations in 2D media (where the $\tilde{E}$ field is polarised perpendicular to the plane of incidence) reduces to the scalar Helmholtz equation, is given in the Appendix Section A.2.

6: In case of the electromagnetic wave transport experiments in 3D random media involving the electric (E) and the magnetic (H) vector fields, it can be assumed that the polarisation state of the scattered electric/magnetic wave field components would be considerably randomised with respect to the polarisation state of the incident wave due to the random scattering.

incident beam, accounting transverse diffusion inside the disorder. The eigenmodes⁷ (defined with respect to the disorder-less region) serves as a basis set (called as the eigenmode basis set) for representing any arbitrary wave mode satisfying the boundary condition within the region. In other words, the linear superposition of the basis wavestates (eigenmodes), weighted by their complex coefficients forming a basis expansion, is used to decompose (or synthesise) any wave pattern observed within the region, with or without the disorder. These eigenmodes could be propagating modes or evanescent modes in general.

7: The term "eigenmode" should not be confused with the term "eigenchannel mode" to be defined later in the chapter. The eigenchannel modes are linear combinations of the eigenmodes.

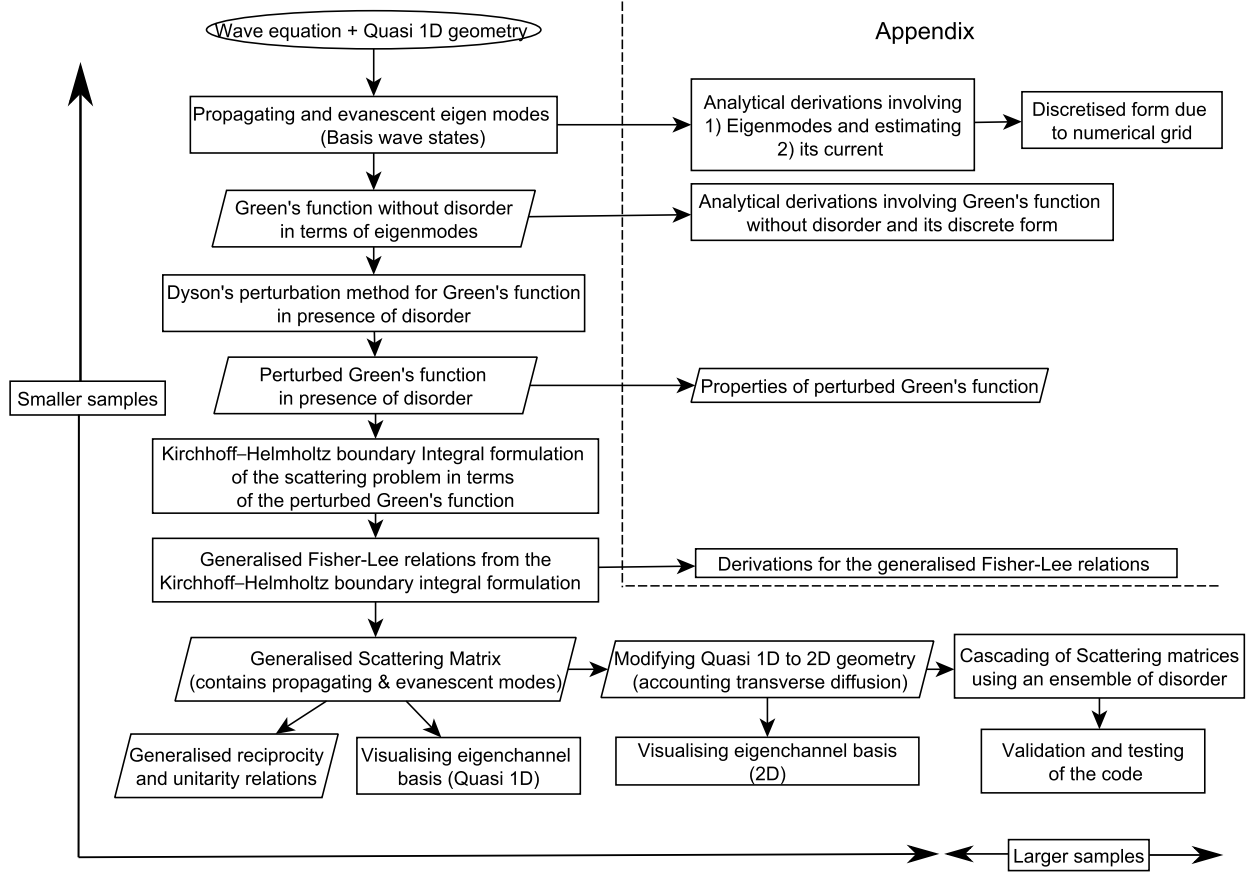


Figure 1.1: The chapter overview is shown. Any digression to the logical flow of the main chapter contents, is provided in the Appendix. The first part of the chapter deals with the smaller samples for visualisation and testing purposes. Towards the end of the chapter, larger samples are obtained using the S matrix cascading method.

It is followed by the definition of the Green's function without any disorder $G_0(r, r_0)$ (also referred as the unperturbed Green's function), in terms of this eigenmode basis set containing both propagating and evanescent eigenmodes. As the Green's function is formed as a linear superposition of the propagating and the evanescent eigenmodes, the Green's function also satisfies the same boundary condition satisfied by the eigenmodes. Once $G_0(r, r_0)$ is known, then the disorder perturbation method using the Dyson's equation, is employed to estimate the Green's function in presence of disorder $G(r, r_0)$, also referred to as the perturbed Green's function. An iterative method involving a block of particles taken together, to solve the Green's function perturbation problem, is described in the thesis. Next, as given in the flowchart, the scattering problem is formulated as the Kirchhoff-Helmholtz boundary integral equation involving the perturbed Green's function. This is particularly convenient

in estimating and visualising the total field in the computational domain due to an incident wave field. It is to be noted that the total field is the superposition of the incident field and the scattered field. As the Kirchhoff–Helmholtz boundary integral formulation of the scattering problem connects 1) the total field in the computational domain, 2) the perturbed Green’s function and 3) the incident wave, the field transmission and the reflection coefficients associated with the transmitted and the reflected waves, can be evaluated. Such a method of estimating the complex reflection and transmission coefficients by matching the reflected and the transmitted fields with the total field estimated can be connected to the formalism of the Fisher-Lee relation[21]. Although the conventional Fisher-Lee relation was published for addressing the electronic conductance involving only the propagating modes, it is contextualised and generalised in this chapter, suiting to the development of wavefront shaping methods containing the evanescent eigenmodes as well. The derivation of the extended/generalised Fisher-Lee relation to estimate the generalised S matrix, forms the corner stone of the flowchart and also of the chapter. The estimated S matrix also satisfies the generalised reciprocity and unitarity relations, involving both propagating and evanescent modes. The rest of the chapter is regarding the estimation of the eigenchannel basis, which involves the singular value decomposition (S.V.D) and the S matrix. Such a change of basis from the eigenmode basis to the eigenchannel basis, is advantageous in understanding the wave transport phenomena in terms of the eigenchannels. These eigenchannels are characterised by their transmission coefficients, ranging from 0 to 1 for the quasi-1D geometry. The statistical aspects of the transmission matrix contained within the S matrix is discussed towards the end of the chapter and also serves the purpose of testing the developed coding framework, with respect to the known random matrix theory results.

1.2 Geometry of the problem and the boundary conditions

First, the slab geometry and the boundary conditions used in this chapter are defined, as shown in the Figure 1.2. In this thesis, there are always reflection (also referred as mirror or Dirichlet) boundary conditions placed along the transverse boundaries ($y = 0$ and $y = W$) so that the wave power doesn’t leak out, crossing the transverse boundaries. The boundaries along the longitudinal dimension (along z) axis are completely open for the wave propagation and the corresponding boundary condition is called as the outgoing boundary condition. Such a confined geometry has the convenience that the total reflection (R) and the total transmission (T) can be estimated with respect to the longitudinal boundaries (Γ_L and Γ_R) as there is no wave flux crossing the transverse boundaries. W indicates the transverse size (along the y axis) of the disorder and L denotes the longitudinal size (along z axis) as shown in the Figure 1.2. In this thesis, the term quasi-1D transport problem implies that $W > L$ with the transverse mirror boundary condition and the incident wave modes have a transverse size of W extending all the way along the slab, exciting the entire slab surface. Later⁸ in the chapter,

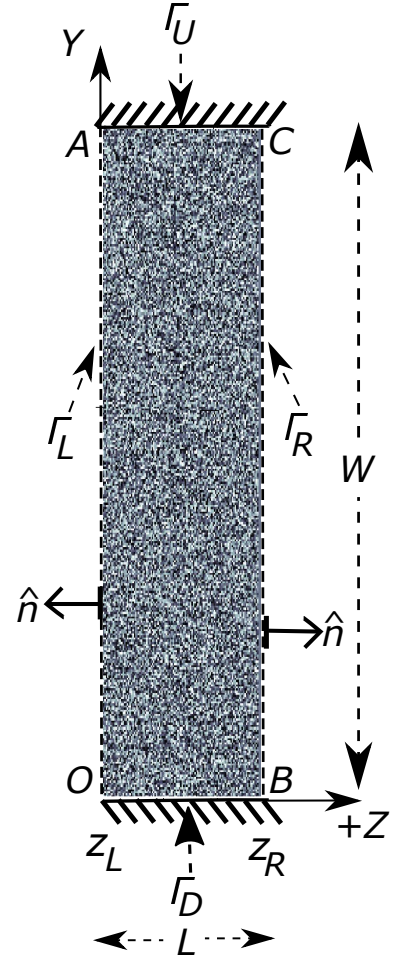


Figure 1.2: The geometry of the scattering problem is given. The boundary around the disorder (AOBCA) is denoted by Γ , which is the union of four boundary segments Γ_L , Γ_D , Γ_R and Γ_U where L stands for left, R stands for right, U stands for up and D for down sides of the disorder. The 2D region enclosed by Γ , is referred to as Ω . The transverse boundaries Γ_U and Γ_D have the reflection(mirror) boundary conditions. The transverse size of the slab is W and the longitudinal thickness is L . Note that the eigenmodes are defined with respect to the same region Ω bounded by AOBC, without any disorder perturbation. Γ_L and Γ_R also serves as the source planes from which, both the propagating and the evanescent eigenmodes are incident onto the disordered slab region.

8: To summarise :

- ▶ Quasi-1D transport problem : Transverse width of the incident wave = $D_{in} = W$, (exciting the entire slab surface along Y axis) and $W \gg L$ (slab medium).
- ▶ 2D transport problem : $D_{in} < W$ and $W > L$.

the 2D transport problem will be addressed such that the incident basis wave modes have a finite beam width $D_{in} < W$, to account for the transverse diffusion within the disorder. Next, the eigenmodes in the context of the quasi-1D transport problem are defined. These eigenmodes are defined with respect to the disorder-less waveguide, without any scatterers present. The relative dielectric constant of the disorder, $\tilde{\epsilon}_r(r)$ is defined as a spatially dependent perturbation $\delta\tilde{\epsilon}_r(r)$, against a spatially independent(uniform) reference (background) dielectric constant value of $\tilde{\epsilon}_r^{ref}$ as given below.

$$\tilde{\epsilon}_r(r) = \tilde{\epsilon}_r^{ref} + \delta\tilde{\epsilon}_r(r) \quad (1.2)$$

Substituting the perturbed disorder in the wave equation 1.1 yields,

$$[\nabla^2 + k_0^2 \mu_r \{\tilde{\epsilon}_r^{ref} + \delta\tilde{\epsilon}_r(r)\}] \tilde{E}(r) = 0, \quad (1.3)$$

If there is no disorder, then the perturbation $\delta\tilde{\epsilon}_r(r) = 0$ and the wave equation for the disorder-less region takes the form

$$[\nabla^2 + k_{ref}^2] \tilde{E}(r) = 0, \quad (1.4)$$

where $k_{ref}^2 = k_0^2 \mu_r \tilde{\epsilon}_r^{ref}$ such that k_{ref} is the wave vector in the spatially uniform reference (background) dielectric medium. As the refractive index $\eta(r) = \sqrt{\tilde{\epsilon}_r(r)}$ and taking $\mu_r = 1$, $k_{ref} = k_0 \eta_{ref}$ where $\eta_{ref} = \sqrt{\tilde{\epsilon}_r^{ref}}$ is the refractive index of reference (background) dielectric medium.

1.3 Propagating and evanescent eigenmodes : The eigenmode basis

The eigenmodes for the quasi-1D geometry can be considered as the basis waves states (without any disorder) such that the modes are independent and orthonormal to each other and satisfies the Helmholtz wave equation with the given boundary conditions. There are two kinds of eigenmodes. 1) The propagating eigenmodes⁹ and 2) the evanescent eigenmodes. The propagating eigenmodes are defined to be existing everywhere in the computational domain. On the other hand, the evanescent eigenmodes emerge-out/inject-in from the disorder surface boundaries Γ_L and Γ_R , and generally die out within few wavelengths from the surface boundaries. Unlike the propagating eigenmodes, an evanescent eigenmode by itself doesn't radiate the wave current (flux) out of the disorder. The evanescent eigenmodes physically exist only in the presence of the disorder and hence don't exist independently in a disorder-less computational domain unless there is a wave source injecting the evanescent wave components into the computational domain. An example for such a situation is the Green's function in the disorder-less region, where the source vicinity has evanescent components associated with it. Nevertheless, examples of the evanescent eigenmodes are plotted for the representational purposes (without any disorder present in the computational domain) as shown in Figure 1.5 and Figure 1.6. These eigenmodes (propagating + evanescent) form a complete basis set such that any arbitrary wave existing inside the region can be expanded/decomposed as a linear

9: Two examples of the propagating eigenmodes are plotted in Figure 1.3 and Figure 1.4, for $m = 3$ and $m = 20$.

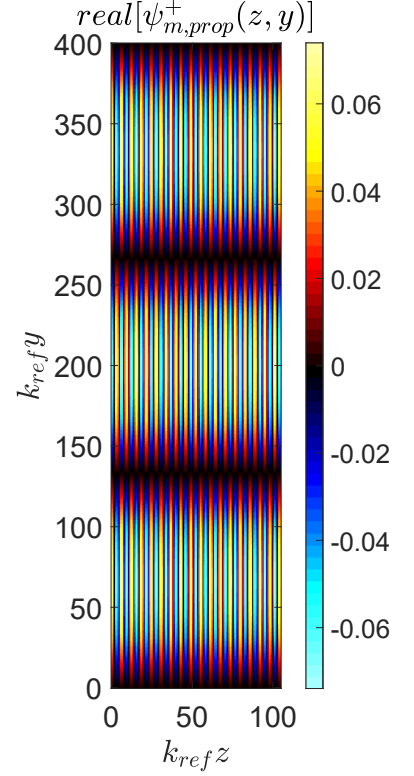


Figure 1.3: The real part of the third propagating eigenmode is shown, where $m = 3$.

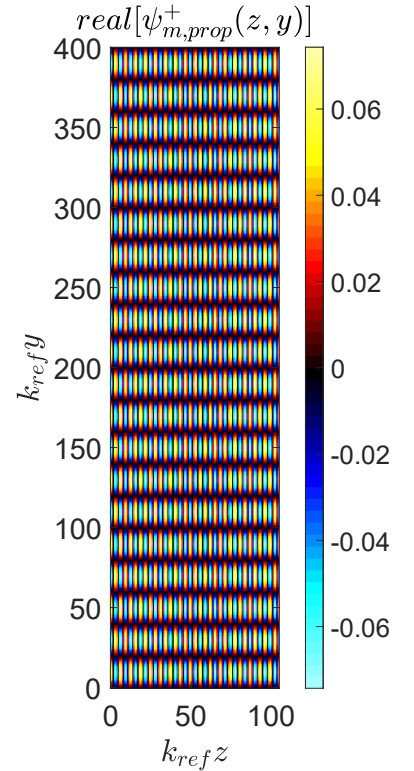


Figure 1.4: The real part of the 20th propagating eigenmode is shown, where $m = 20$.

superposition of the eigenmodes with their corresponding complex basis expansion coefficients. For a given geometry as shown in Figure 1.2 with transverse size W , there exist a finite number $(2\eta_{ref}W/\lambda_0)$ of propagating eigenmodes and an infinite number of evanescent eigenmodes. For the computational purposes, all propagating modes are accounted, while the number of evanescent modes are truncated for a pre-defined number. Two examples of evanescent eigenmodes are plotted in Figure 1.5 and Figure 1.6. The relevance of using this eigenmode basis wave set is that any arbitrary wave (including the Green's function) can be expressed as a basis expansion of the individual eigenmodes with their corresponding complex expansion coefficients. The right travelling and the left travelling propagating eigenmodes $\psi_m^\pm$ are defined with respect to the same coordinate axis YOZ given in the Figure 1.2 as the following (as a variable separable form)

The right travelling propagating eigenmodes (along $+z$ direction)

$$\psi_{m,prop}^+(z, y) = \Phi_{m,prop}^+(z)\chi_m(y) \quad (1.5)$$

where $\Phi_{m,prop}^+(z) = \frac{1}{\sqrt{k_z^{(m)}}}e^{+ik_z^{(m)}z}$ and $\chi_m(y) = \sqrt{\frac{2}{W}}\sin(k_y^{(m)}y)$

The left traveling propagating eigenmodes (along $-z$ direction)

$$\psi_{m,prop}^-(z, y) = \Phi_{m,prop}^-(z)\chi_m(y) \quad (1.6)$$

where $\Phi_{m,prop}^-(z) = \frac{1}{\sqrt{k_z^{(m)}}}e^{-ik_z^{(m)}z}$ and $\chi_m(y)$ same as before.

such that $k_y^{(m)} = m\pi/W$ is the magnitude of the transverse wave vector component of the m^{th} eigenmode along the y direction and $k_z^{(m)}$ is the magnitude of the longitudinal wave vector component of the m^{th} eigenmode along the z direction. (m) as the superscript of $k_y^{(m)}$ denotes the integer index number for the m^{th} wave vector. $+$ symbol as a superscript of $\Phi_{m,prop}^+(z, y)$ and $\psi_{m,prop}^+(z, y)$ denote the wave propagation along $+z$ direction (from the left to the right of the computational domain) and $-$ symbol denote the propagation along $-z$ direction (from the right to the left). The function $\chi_m(y)$ is the transverse component of the eigenmode satisfying the mirror boundary conditions and it obeys the orthogonality relationship $\langle \chi_m(y) | \chi_n(y) \rangle = \delta_{kron}(m, n)$, where δ_{kron} is the Kronecker delta function (for more details refer Appendix Section A.3.2).

The eigenmodes satisfy the Helmholtz equation

$$[\nabla^2 + k_{ref}^2]\psi_m(z, y) = 0, \quad (1.7)$$

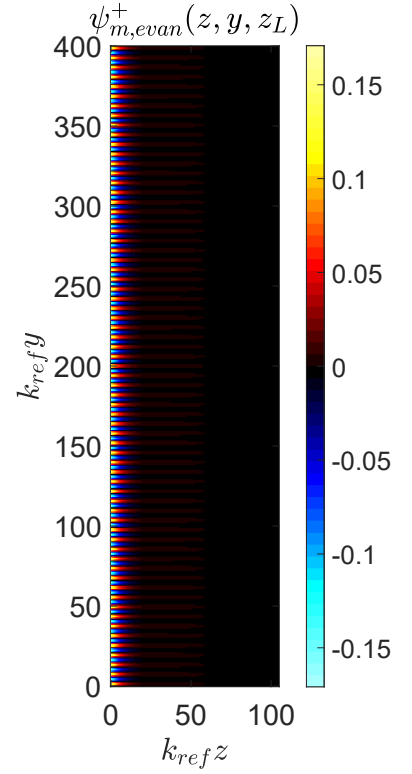


Figure 1.5: The third evanescent eigenmode emerging from Γ_L , propagating rightwards is shown. Attenuation towards the right side can be observed.

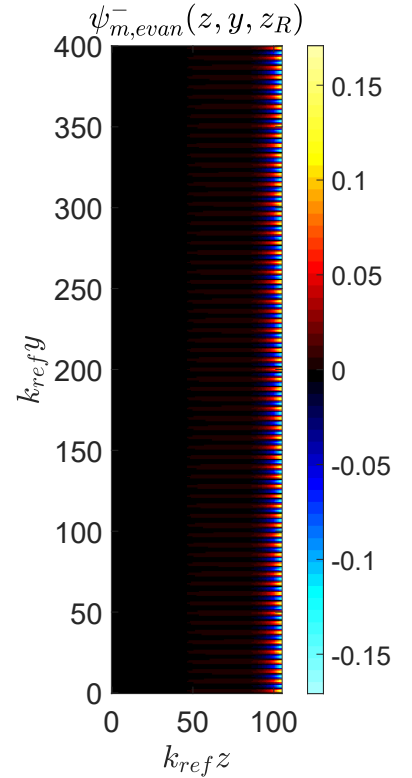


Figure 1.6: The third evanescent eigenmode emerging from Γ_R , propagating leftwards is shown.

such that $(k_z^{(m)})^2 + (k_y^{(m)})^2 = k_{ref}^2$, which is the dispersion relation.

The wave vector magnitude components $k_y^{(m)}$ and $k_z^{(m)}$ obey the dispersion relation.¹⁰ Here, only the scenario of monochromatic wave transport through a stationary disorder is studied and hence k_{ref} is fixed as a constant due to the reason that the ω value is fixed. For the evanescent eigenmodes, $k_z^{(m)} = \sqrt{k_{ref}^2 - (k_y^{(m)})^2} = ik_{z,evan}^{(m)}$ are purely imaginary, where the real number $k_{z,evan}^{(m)} = \sqrt{(k_y^{(m)})^2 - k_{ref}^2}$. Hence, the evanescent eigenmodes defined with respect to Γ_L and Γ_R (refer Figure 1.5 and Figure 1.6) are given as the following.

The evanescent eigenmodes defined with respect to Γ_L where the wave emerges to left (-) or right (+) of Γ_L

$$\psi_{m,evan}^{\pm}(z, y) = \Phi_{m,evan}^{\pm}(z, z_L) \chi_m(y) \quad (1.8)$$

$$\text{where } \Phi_{m,evan}^{\pm}(z, z_L) = \frac{1}{\sqrt{|k_z^{(m)}|}} e^{-ik_z^{(m)}|z-z_L|} = \frac{1}{\sqrt{k_{z,evan}^{(m)}}} e^{-k_{z,evan}^{(m)}|z-z_L|}$$

The evanescent eigenmodes defined with respect to Γ_R where the wave emerges to left (-) or right (+) of Γ_R

$$\psi_{m,evan}^{\pm}(z, y) = \Phi_{m,evan}^{\pm}(z, z_R) \chi_m(y) \quad (1.9)$$

$$\text{where } \Phi_{m,evan}^{\pm}(z, z_R) = \frac{1}{\sqrt{|k_z^{(m)}|}} e^{-ik_z^{(m)}|z-z_R|} = \frac{1}{\sqrt{k_{z,evan}^{(m)}}} e^{-k_{z,evan}^{(m)}|z-z_R|}$$

One may note that both the propagating and the evanescent eigenmodes ψ_m include a normalisation factor $1/\sqrt{|k_z^{(m)}|}$. The reason for including such a normalisation factor is explained in the sidenote¹¹ after defining the wave current density (also known as flux density) associated with eigenmodes. Let $\vec{J}(r)$ denote the flux density vector field associated with the scalar wave equation.¹²

The flux (current) density of the m^{th} wave eigenmode

$$\begin{aligned} \vec{J}^{(m)}(z, y) &= \frac{1}{2i} \{ \psi_m^* \nabla \psi_m - \psi_m \nabla \psi_m^* \} = \text{Imag}[\psi_m^* \nabla \psi_m] \\ &= J_z^{(m)}(z, y) \hat{e}_z + J_y^{(m)}(z, y) \hat{e}_y \end{aligned} \quad (1.10)$$

where $*$ denotes complex conjugation, Imag denotes imaginary part of, $\hat{e}_z$ and $\hat{e}_y$ the unit vectors along z and y . There is no flux crossing the mirror reflection boundaries Γ_U and Γ_D along $\hat{e}_y$ (boundaries are shown in Figure 1.2). The surface integrated flux density normal to $\hat{e}_z$

10: The relation $(k_y^{(m)})^2 + (k_z^{(m)})^2 = k_{ref}^2$ is called as the "dispersion relation" as it relates the y component $k_y^{(m)}$ and z component $k_z^{(m)}$ of the wave vector with respect to the fixed temporal frequency of the wave as $k_{ref} = 2\pi\eta_{ref}/\lambda_0 = \omega\eta_{ref}/c$.

11: For the propagating modes, the normalisation factor $\frac{1}{\sqrt{k_z^{(m)}}}$ ensures that the flux (the current) component flowing through a given boundary region Γ_L or Γ_R , perpendicular to the surface is unity as given in the equation 1.11. Such a flux normalisation is essential in defining the S matrix later in the chapter, as it is required as a standardisation condition that all the propagating basis modes inject unit flux normal to the boundary under consideration. For the evanescent modes, as there is no flux crossing the boundaries, physically there is no need for defining a normalisation factor. Nevertheless, a normalisation factor $\frac{1}{\sqrt{|k_z^{(m)}|}} = \frac{1}{\sqrt{k_{z,evan}^{(m)}}}$ is included in the definition for the evanescent eigenmodes. This is mainly for the numerical convenience of making the propagating modes and the evanescent modes, of the same order. If $\frac{1}{\sqrt{k_{z,evan}^{(m)}}}$ is not included in the definition of the evanescent eigenmodes, then the evanescent modes will be several orders larger compared to the propagating modes, leading to numerical multiplication precision errors while estimating the S matrix.

12: Refer page 84 of [30] or [31] or equation 2.39 of [19] for the expression of the current density.
[30]: Frish (1968), 'Wave propagation in random media'

[31]: Cazé et al. (2015), 'Diagrammatic and asymptotic approaches to the origins of radiative transport theory: tutorial'

[19]: Carminati et al. (2021), *Principles of Scattering and Transport of Light*

direction on Γ_L or Γ_R ,

$$(flux)_m = \int_{\Gamma} J_z^{(m)}(z, y) \hat{e}_z \cdot \hat{e}_z dy = 1 \text{ for the propagating modes} \\ = 0 \text{ for the evanescent modes} \quad (1.11)$$

where $z, y \in \Gamma_L$ or Γ_R . Refer the Appendix Section A.4 for the proof that the net flux crossing a boundary surface Γ , is unity for the propagating eigenmodes. For the evanescent eigenmodes, ψ_m is a real expression and hence according to the equation 1.10, the flux is zero.

1.3.1 Discrete form of eigenmodes on a computational grid

For representing the analytical functions presented in the chapter as a function of z and y while coding, numerical grids (shown in Figure 1.7), similar to the ones used in the finite difference methods[32], are used. These numerical grids always have a finite grid cell size Δ_z and Δ_y . For the analytical expressions given in the chapter to be exact on the grid, Δ_z and Δ_y have to tend to zero, which is practically impossible due to the memory and the computational processing capacity limitations. Hence, Δ_z and Δ_y take a trade-off size such that they are small enough to resolve waves on the grids (especially the evanescent eigenmodes), but not too small consuming all the available memory and the processing capacity. For a review on the influence of grid sizes on the accuracy of finite difference schemes and its effect on the dispersion relationship, refer [33]. Let there be N_z grid points/nodes along the z direction and N_y along the y direction so that there are $N_z N_y$ grid points with the grid spacing being Δ_z and Δ_y . Hence, the longitudinal size of the region is $(N_z - 1)\Delta_z$ and transverse size is $(N_y - 1)\Delta_y$. Let $z_i = [1 : N_z]$ and $y_j = [1 : N_y]$ which are represented in the Matlab notation system.¹³ Then, the discrete z values are given as $z = (z_i - 1)\Delta_z$ and $y = (y_j - 1)\Delta_y$ which form an array of numbers for z and y . In addition to that, $W = (N_y - 1)\Delta_y$. Therefore, the analytical form the eigenmodes (given in the equations 1.5 and 1.6) take the following discrete¹⁴ form (For the derivations, refer to the Appendix Section A.6).

The discrete representation of eigenmodes on a computational grid

$$\psi_{m,prop}^{\pm}(z_i, y_j) = \frac{\Phi_m^{\pm}(z_i)}{\sqrt{\frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z}}} e^{\pm i k_z^{(m)} \Delta_z (z_i - 1)} \chi_m(y_j) \quad (1.12)$$

Here,

$$\chi_m(y_j) = \sqrt{\frac{2}{W}} \sin\{k_y^{(m)} \Delta_y (y_j - 1)\} \quad (1.13)$$

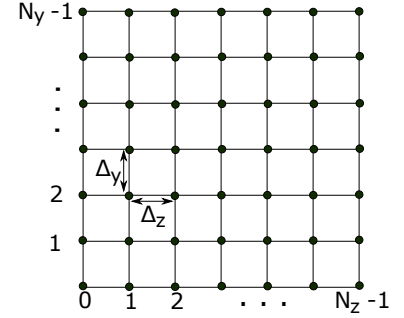


Figure 1.7: Schematic for a typical computational grid of size $[N_y \times N_z]$ is shown.

[32]: Taflove et al. (2005), *Computational electrodynamics: the finite-difference time-domain method*

[33]: Harari et al. (1995), 'Accurate finite difference methods for time-harmonic wave propagation'

13: In Matlab, the operator : gives integer step values between 1 and N_z or N_y

14: The discrete form of eigenmodes approaches the continuous analytic form, upon taking the limit $\Delta_z \rightarrow 0$ and $\Delta_y \rightarrow 0$.

Note that the $\lim_{\Delta_z \rightarrow 0} \frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z} = k_z^{(m)}$. While implementing the coding for the modelling, the product $k_y^{(m)} \Delta_y$ is treated as a single term (dimensionless) of the order of unity, mainly to avoid the precision errors, while evaluating χ_m . This is because $k_y^{(m)}$ would be very large in magnitude compared to Δ_y . Similarly, $k_z^{(m)} \Delta_z$ is also treated as a single variable, of the order of unity.

with the discrete form of orthogonality relationship being

$$\sum_{y_j} \chi_m(y_j) \chi_n(y_j) \Delta_y = \delta_{kron}(m, n) \quad (1.14)$$

Similarly, for the evanescent modes given in equation 1.8 and 1.9,

$$\Phi_{m, evan}^\pm(z, z_{L/R}) = \frac{1}{\sqrt{|k_z^{(m)}|}} e^{-ik_z^{(m)}|z-z_{L/R}|} = \frac{1}{\sqrt{k_{z, evan}^{(m)}}} e^{-k_{z, evan}^{(m)}|z-z_{L/R}|} \text{ gets}$$

replaced by

$$\Phi_{m, evan}^\pm(z_i, z_{iL/R}) = \frac{1}{\sqrt{\frac{\sin(|k_z^{(m)}| \Delta_z)}{\Delta_z}}} e^{-k_{z, evan}^{(m)} \Delta_z |z_i - z_{iL/R}|} \quad (1.15)$$

L/R as a subscript denotes the left(L) or the right(R). Substituting the discrete form of eigenmodes in the wave equation, the discrete version of the dispersion relation (For derivations, refer to the Appendix Section A.7) is obtained, as given below.

The discrete dispersion relationship

$$\frac{4}{\Delta_z^2} \sin^2 \left(\frac{k_z^{(m)} \Delta_z}{2} \right) + \frac{4}{\Delta_y^2} \sin^2 \left(\frac{k_y^{(m)} \Delta_y}{2} \right) = k_{ref}^2 \quad (1.16)$$

Set $\Delta_z = \Delta_y = \Delta$, then the above given equation can be re-written as

$$2 - \cos(k_z^{(m)} \Delta) - \cos(k_y^{(m)} \Delta) = \frac{(k_{ref} \Delta)^2}{2} \implies k_z^{(m)} \Delta = \cos^{-1} \left\{ 2 - \cos(k_y^{(m)} \Delta) - \frac{(k_{ref} \Delta)^2}{2} \right\} \quad (1.17)$$

The discretised dispersion relationship is used to evaluate $k_z^{(m)} \Delta$ for a given $k_y^{(m)} \Delta$. For the propagating eigenmodes containing real $k_z^{(m)}$, the argument inside $\cos^{-1}$ has to remain between $(-1, 1)$ ¹⁵ implying $0 < (k_{ref} \Delta) \leq 2\sqrt{2}$ in free space. For practical coding purposes, especially in the presence of disorder and the evanescent modes, $k_{ref} \Delta < 1$ such that it resolves the evanescent eigenmode with the highest¹⁶ transverse spatial frequency, $k_{y, max}^{(m)}$. Hence, Δ is chosen such that $k_{y, max}^{(m)} \Delta = 1$. Next, the analytical boundary conditions satisfied by the eigenmodes at Γ_L or Γ_R is given as the following.

1.3.2 Homogeneous boundary conditions for the propagating and the evanescent eigenmodes

For both the boundaries Γ_L or Γ_R in the slab geometry (shown in figure Figure 1.2), the following homogeneous¹⁷ boundary condition holds for the propagating eigenmodes.

15: Simplifying the inequality relationship for having $k_{ref} \Delta$ as a real term (applicable only for the propagating modes),

$$-1 \leq 2 - \cos(k_y^{(m)} \Delta) - \frac{(k_{ref} \Delta)^2}{2} \leq 1 \implies 3 - \cos(k_y^{(m)} \Delta) \geq \frac{(k_{ref} \Delta)^2}{2} \geq 1 - \cos(k_y^{(m)} \Delta)$$

As $\cos(k_y^{(m)} \Delta)$ fluctuates between $(-1, 1)$, $0 < (k_{ref} \Delta) \leq 2\sqrt{2}$, in free space and involving only propagating modes. In presence of disorder and also to include evanescent modes, $k_{ref} \Delta < 1$ such that it well-resolves the evanescent eigenmode with the highest transverse spatial frequency.

16: Analytically speaking, there are infinite number of evanescent eigenmodes possible. However in the coding framework, the number of evanescent modes are truncated at a certain number (For example, 30 evanescent modes) in this chapter. Larger the number of evanescent modes, smaller should be the Δ value for resolving the evanescent modes with very high spatial frequencies, thereby increasing the computational burden with respect to the memory and the processing power.

17: The word ‘‘homogeneous’’ implies that R.H.S of the boundary condition involving $\psi_m^\pm(z, y)$ doesn’t involve an extra source wave term (is zero).

Homogeneous boundary conditions for the propagating eigenmodes

$$\frac{\partial}{\partial z} \psi_{m,prop}^{\pm}(z, y)|_{(z,y) \in \Gamma_{L/R}} \mp i k_z^{(m)} \psi_{m,prop}^{\pm}(z, y)|_{(z,y) \in \Gamma_{L/R}} = 0 \quad (1.18)$$

For the evanescent waves, the homogeneous boundary conditions need to be treated separately as given below. The main purposes^{18,19} of defining the eigenmodes and their associated homogeneous boundary conditions are given in the sidenotes.

Homogeneous boundary conditions for the evanescent eigenmodes

a) Let $z = z_L + \delta_z$ where $\delta_z \rightarrow 0^+$ (Slightly inside the box AOBC (shown in Figure 1.2) closer to Γ_L denoted as Γ_L^+). The right going evanescent wave closer to Γ_L , is then given by

$$\psi_{m,evan}^+(z, y) = \frac{1}{\sqrt{k_{z,evan}^{(m)}}} e^{-(z-z_L)k_{z,evan}^{(m)}} \quad (1.19)$$

$$\frac{\partial}{\partial z} \psi_{m,evan}^+(z, y)|_{(z,y) \in \Gamma_L^+} + k_{z,evan}^{(m)} \psi_{m,evan}^+(z, y)|_{(z,y) \in \Gamma_L^+} = 0 \quad (1.20)$$

b) When $z = z_L - \delta_z$ (Slightly outside the box AOBC closer to Γ_L denoted by Γ_L^-). The left going evanescent wave closer to Γ_L is

$$\psi_{m,evan}^-(z, y) = \frac{1}{\sqrt{k_{z,evan}^{(m)}}} e^{+(z-z_L)k_{z,evan}^{(m)}} \quad (1.21)$$

$$\frac{\partial}{\partial z} \psi_{m,evan}^-(z, y)|_{(z,y) \in \Gamma_L^-} - k_{z,evan}^{(m)} \psi_{m,evan}^-(z, y)|_{(z,y) \in \Gamma_L^-} = 0 \quad (1.22)$$

Similarly, on the boundary at right side Γ_R ,

c) Let $z = z_R + \delta_z$ (Slightly outside the box AOBC closer to Γ_R denoted as Γ_R^+). The right going evanescent wave closer to Γ_R , is then given by

$$\psi_{m,evan}^+(z, y) = \frac{1}{\sqrt{k_{z,evan}^{(m)}}} e^{-(z-z_R)k_{z,evan}^{(m)}} \quad (1.23)$$

$$\frac{\partial}{\partial z} \psi_{m,evan}^+(z, y)|_{(z,y) \in \Gamma_R^+} + k_{z,evan}^{(m)} \psi_{m,evan}^+(z, y)|_{(z,y) \in \Gamma_R^+} = 0 \quad (1.24)$$

d) When $z = z_R - \delta_z$ (Slightly inside the box AOBC closer to Γ_R denoted by Γ_R^-). The left going evanescent wave closer to Γ_R is

$$\psi_{m,evan}^-(z, y) = \frac{1}{\sqrt{k_{z,evan}^{(m)}}} e^{+(z-z_R)k_{z,evan}^{(m)}} \quad (1.25)$$

$$\frac{\partial}{\partial z} \psi_{m,evan}^-(z, y)|_{(z,y) \in \Gamma_R^-} - k_{z,evan}^{(m)} \psi_{m,evan}^-(z, y)|_{(z,y) \in \Gamma_R^-} = 0 \quad (1.26)$$

Therefore, the homogeneous boundary conditions for both the propagating and the evanescent eigenmodes, can then be combined as the following

18: The purpose of defining the eigenmode basis set. Any arbitrary wave $\tilde{E}(z, y)$ (or Green's function) that exist in the computational domain could be written as a linear superposition of $\psi_m^+(z, y)$ and $\psi_m^-(z, y)$. As an example, for wave incident only from the left side of the disorder, the outgoing transmitted wave from a random medium (on the right side of the disorder) could be expressed only in terms of $\psi_m^+(z, y)$ eigenmodes. On the contrary, the total wave on the incident side (left side) of the sample would contain both reflected and the incident wave, which requires the total wave to be expanded in terms of both $\psi_m^+(z, y)$ and $\psi_m^-(z, y)$ eigenmodes. As any arbitrary wave $\tilde{E}(z, y)$ can be written in terms of eigenmodes $\psi_m^{\pm}(z, y)$ as a coefficient expansion, the homogeneous boundary conditions given in equation 1.27 are also applicable for the total wave $\tilde{E}(z, y)$.

19: The purpose of defining the homogeneous eigenmode boundary conditions at Γ_L and Γ_R . The main use of the eigenmode boundary conditions is to simplify the Kirchhoff-Helmholtz boundary integral formulation of the scattering problem, to be defined later in the chapter. The boundary integral formulation involves the Green's function and the total field values along with their spatial derivatives, at the boundaries Γ_L and Γ_R . As the total field and the Green's function in presence of disorder can be expressed as a basis expansion involving eigenmodes, the $\frac{\partial}{\partial z}$ derivatives in the boundary integral (involving the eigenmodes) can be simplified using the boundary conditions.

Combined homogeneous boundary conditions for both the propagating and the evanescent eigenmodes

$$\frac{\partial}{\partial z} \psi_m^\pm(z, y) \mp i k_z^{(m)} \psi_m^\pm(z, y) = 0, \quad (1.27)$$

where $k_z^{(m)} = i k_{z, \text{evan}}^{(m)}$ for the evanescent eigenmodes.

The discussions regarding the eigenmodes conclude here and in the following sections, the essential concepts regarding the Green's function are reviewed.

1.4 Green's function and the Dyson's perturbation method

The frequency domain Green's function can be considered as the wave impulse response at a field evaluation point r due to a Dirac delta²⁰ source (continuous in time), $\delta(r, r_0)$ placed at r_0 . In the wave transport theory, there are two kinds of Green's functions. The first kind is the Green's function $G_0(r, r_0)$ (note the subscript 0) in a homogeneous (uniform) medium **without** any scatterers or disorder. The second kind would be the Green's function $G(r, r_0)$, to be evaluated **in the presence** of the disorder. To give a physical intuition to the concept of Green's function, the unperturbed Green's function $G_0(r, r_0)$ is analytically computed and plotted in Figure 1.8, at various field positions r and a given source at r_0 . Once $G_0(r, r_0)$ is evaluated analytically, then $G(r, r_0)$ (in the presence of disorder) can be estimated by using $G_0(r, r_0)$ together with the Dyson's equation, which will be explained towards the end of this section. Before getting into the details of the Dyson's equation and the perturbation theory associated with it, Green's functions (both $G_0(r, r_0)$ and $G(r, r_0)$) have to be defined as the following.

Consider a general differential equation

$$\mathcal{L} \tilde{E}(r) = \tilde{S}(r) \quad (1.28)$$

where $\mathcal{L}$ is a differential operator acting on $\tilde{E}(r)$ and $\tilde{E}(r)$ can be considered as a function²¹ which needs to be solved for a given source term $\tilde{S}(r)$. In the context of this thesis, let $\mathcal{L}$ represent the Helmholtz operator (without the disorder) ie. $\mathcal{L} = [\nabla^2 + k_{ref}^2]$. For a given arbitrary source $\tilde{S}(r)$, $\tilde{E}(r)$ could be solved as the following convolution²²

$$\tilde{E}(r) = \int_{r_1} G_0(r, r_1) \tilde{S}(r_1) dr_1, \quad (1.29)$$

where $G_0(r, r_0)$ is the Green's function for the operator $\mathcal{L}$ such that

$$\mathcal{L} G_0(r, r_0) = \delta(r - r_0) \quad (1.30)$$

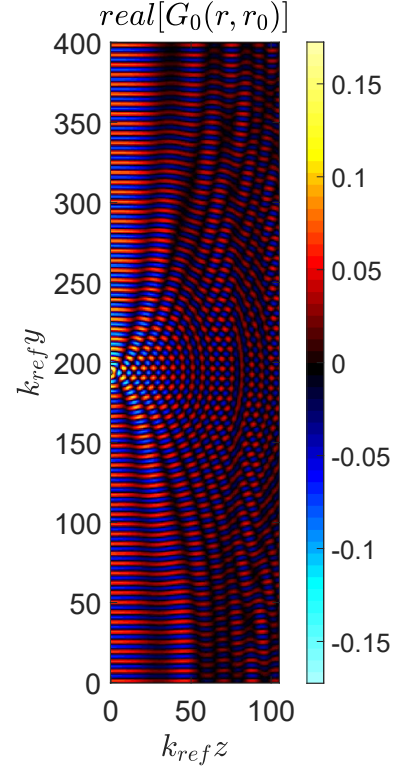


Figure 1.8: The unperturbed Green's function $G_0(z, y, z_0, y_0)$ is shown. The real part of $G_0(z, y, z_0, y_0)$ is plotted using the equation 1.40 for (z, y) , where the source location $(k_{ref} z_0, k_{ref} y_0) = (0, 194.21)$. In addition to all the propagating modes, 30 evanescent eigenmodes are also used in implementing the equation 1.40, while coding.

20: Refer section 15 : "The δ function" of [34] for details.

21: The time or frequency dependence on both $\tilde{E}(r)$ and $\tilde{S}(r)$ is harmonic in nature with the factor $e^{-i\omega t}$, implying $\tilde{E}(r, \omega) = \tilde{E}(r)e^{-i\omega t}$ and $\tilde{S}(r, \omega) = \tilde{S}(r)e^{-i\omega t}$

22: In 2D, $r_1 \in \mathbb{R}^2$ and $\int_{r_1} dr_1$ denotes $\int_z \int_y dz dy$ and in 3D, $r_1 \in \mathbb{R}^3$ and $\int_{r_1} dr_1$ means $\int_x \int_y \int_z dx dy dz$.

Next, consider the Helmholtz equation for Green's function in the presence of disorder.

$$[\nabla^2 + k_0^2 \mu_r \tilde{\epsilon}_r(r)]G(r, r_0) = \delta(r - r_0) \quad (1.31)$$

Express $\tilde{\epsilon}_r(r)$ as a spatially dependent perturbation $\delta\epsilon_r(r)$ (as shown in Figure 1.9), against a uniform background reference dielectric constant value of $\tilde{\epsilon}_r^{ref}$ independent of r [35, 36].

$$\tilde{\epsilon}_r(r) = \tilde{\epsilon}_r^{ref} + \delta\epsilon_r(r) \quad (1.32)$$

Substituting the perturbation in equation 1.31,

$$[\nabla^2 + k_0^2 \mu_r \{\tilde{\epsilon}_r^{ref} + \delta\epsilon_r(r)\}]G(r, r_0) = \delta(r - r_0), \quad (1.33)$$

which could be re-arranged to obtain

$$[\nabla^2 + k_{ref}^2]G(r, r_0) = \delta(r - r_0) + V(r)G(r, r_0) \quad (1.34)$$

where $V(r) = -k_0^2 \mu_r \delta\epsilon_r(r)$ is the scattering potential and $k_{ref}^2 = k_0^2 \mu_r \tilde{\epsilon}_r^{ref}$ is the wave vector in the uniform reference (background) dielectric medium. On comparing equation 1.34 with that of the general scenario given in equation 1.28, the following is obtained.

$$\underbrace{[\nabla^2 + k_{ref}^2]}_{\mathcal{L}} \underbrace{G(r, r_0)}_{\tilde{E}} = \underbrace{\delta(r - r_0) + V(r)G(r, r_0)}_{\tilde{S}(r)} \quad (1.35)$$

In addition to that, comparing with equation 1.30 gives

$$\underbrace{[\nabla^2 + k_{ref}^2]}_{\mathcal{L}} \underbrace{G_0(r, r_0)}_{G_0} = \delta(r - r_0) \quad (1.36)$$

Therefore, $G(r, r_0)$ could be solved, similarly to that of equation 1.29

$$\begin{aligned} G(r, r_0) &= \int_{r_1} G_0(r, r_1) \left\{ \underbrace{\delta(r_1 - r_0) + V(r_1)G(r_1, r_0)}_{\tilde{S}(r_1)} \right\} dr_1 \\ &= \int_{r_1} G_0(r, r_1) \delta(r_1 - r_0) dr_1 + \int_{r_1} G_0(r, r_1) V(r_1) G(r_1, r_0) dr_1 \end{aligned} \quad (1.37)$$

Using the sifting property of the Dirac delta function on the first term of R.H.S, the well-known Dyson's equation²³ for the Green's function in the disordered media is obtained, as given below for $G(r, r_0)$.

Dyson's equation for Green's function perturbation

$$G(r, r_0) = G_0(r, r_0) + \int_{r_1} G_0(r, r_1) V(r_1) G(r_1, r_0) dr_1 \quad (1.38)$$

[35]: Martin et al. (1994), 'Iterative scheme for computing exactly the total field propagating in dielectric structures of arbitrary shape'

[36]: Martin et al. (1995), 'Generalized field propagator for electromagnetic scattering and light confinement'

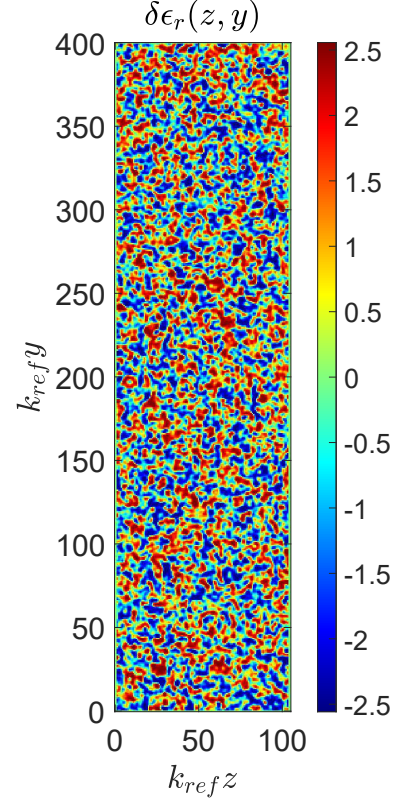


Figure 1.9: An example for a random disorder realisation $\delta\epsilon_r(r)$ (refer equation 1.32) is shown. Here, $k_{ref}L = 101.5368$ and $k_{ref}W = 399.7005$ such that the wave vector for the background medium is $k_{ref} = 2\pi\eta_{ref}/\lambda$ and $\eta_{ref} = 1.9$. The number of grid points used for the sample is $N_y \times N_z = 497 \times 131 = 65,107$. This sample is a smaller sample, to be mainly used for visualising the fields. Later in the chapter, larger samples will be obtained by the S matrix cascade rule. Here, $k_{ref}\Delta_z = k_{ref}\Delta_y = k_{ref}\Delta = 0.8058$ to include 30 evanescent eigenmodes, in addition to the 130 propagating eigenmodes. The disorder exists two unit cells ($k_{ref}2\Delta$) away from the left and the right boundaries Γ_L and Γ_R . The disorder shown is a spatially correlated disorder with the dimensionless spatial correlation length $k_{ref}l_c = 1.9726$ (along z axis). Various aspects of the disorder correlation and the detailed method used to generate it, is given in Chapter 2. The same disorder is used for all the results of this chapter, until Section 1.8.

²³: Refer chapter 3.2 of [37], [35] or page 105 of [30]

The Dyson's equation has an iterative structure that the solution $G(r, r_0)$ appears both in the L.H.S and in the R.H.S of equation 1.38. Various numerical schemes [35, 36, 38] exist for solving $G(r, r_0)$ using the Dyson's equation. As hinted before, the unique analytical or numerical form of the Green's functions, is dependent upon the boundary conditions determined by the geometry of the problem. Before moving into the details of the numerical implementation for solving $G(r, r_0)$, first $G_0(r, r_0)$ needs to be evaluated for a geometry as shown in Figure 1.9, without any disorder present. The analytical expression for $G_0(r, r_0)$ where $r_0 \in \mathcal{R}^2$ and the wave polarised along X axis (perpendicular to YZ plane in the direction of variation of dielectric fluctuations), is given as the following.

1.4.1 Unperturbed Green's function $G_0(r, r_0)$ without the presence of disorder

The analytical expression[39] involving an infinite summation²⁴ for $G_0(r, r_0)$ in 2D for a geometry as shown in Figure 1.9, is given as the following. (For the analytic derivation consistent with the sign conventions used in this thesis, refer to the Appendix Section A.3.)

Unperturbed Green's function

$$G_0(z, y, z_0, y_0) = \sum_{m=1}^{\infty} G_0^{(m)}(z, y, z_0, y_0) \\ = \sum_{m=1}^{\infty} \underbrace{\frac{1}{2ik_z^{(m)}} e^{ik_z^{(m)}|z-z_0|} \sqrt{\frac{2}{W}} \sin(k_y^{(m)}y) \sqrt{\frac{2}{W}} \sin(k_y^{(m)}y_0)}_{G_0^{(m)}(z, y, z_0, y_0)} \quad (1.39)$$

where $k_y^{(m)} = m\pi/W$ and $(k_z^{(m)})^2 = k_{ref}^2 - (k_y^{(m)})^2$. $k_z^{(m)}$ is real for the propagating waves and $k_z^{(m)} = ik_{z,evan}^{(m)}$ (imaginary) for evanescent waves as given before.

[39]: Felsen et al. (2004), 'Wave propagation inside a two-dimensional perfectly conducting parallel-plate waveguide: Hybrid ray-mode techniques and their visualizations'

24: Although the summation in the equation 1.39 runs from $m = 1$ to a large number, the summation is truncated such that it includes all the propagating modes ($M_{prop} \approx 2\eta_{ref}W/\lambda$ propagation modes in 2D and $M_{prop} \approx (k_{ref}W)^2$ in 3D) and a certain truncation number of evanescent modes (M_{evan} evanescent modes). M_{evan} is taken as 30 in this chapter.

25: As the analytical form of $G_0(r, r_0)$ needs to be implemented on a numerical grid with finite grid size Δ_z and Δ_y , the discrete definition of eigenmodes given in equation 1.12 are used for both the propagating and the evanescent terms contained in the analytical expression for $G_0(r, r_0)$.

While implementing the code on a numerical grid, the discrete form²⁵ of $G_0(r, r_0)$ will be used, given as the following.

Discrete form of unperturbed Green's function on a grid

$$G_0(z_i, y_j, z_{0i}, y_{0j}) = \sum_{m=1}^{\infty} d_m e^{i|k_z^{(m)} \Delta_z (z_i - z_{0i})|} \sqrt{\frac{2}{W}} \sin(k_y^{(m)} \Delta_y (y_j - 1)) \sqrt{\frac{2}{W}} \sin(k_y^{(m)} (y_{0j} - 1)) \quad (1.40)$$

where

$$d_m = \begin{cases} \frac{1}{2i \left(\frac{\sin(k_z^m \Delta z)}{\Delta z} \right)}, & \text{if propagating modes are involved } m \leq M_{prop} \\ \frac{1}{-2 \left(\frac{\sin(k_z^m \Delta z)}{\Delta z} \right)}, & \text{if evanescent modes are involved } m > M_{prop} \end{cases} \quad (1.41)$$

Until now, $G_0(r, r_0)$ the unperturbed Green's function was discussed. In the following section, estimation of the Green's function $G(r, r_0)$ in presence of disorder, using $G_0(r, r_0)$ and the Dyson's equation, is provided.

1.4.2 Numerical estimation of the perturbed Green's function $G(r, r_0)$

On a $[N_y \times N_z]$ grid domain, for different source position indices (j) and field position indices (i), Green's functions (say the unperturbed $G_0(z_i, y_i, z_0, y_0)$), can be represented as a 2D matrix of size $[N_z N_y \times N_z N_y]$. Let $G_0(z_i, y_i, z_0, y_0)$ be represented as $G_{ij}^{(0)}$ where both the indices i and j could generally take the value $[1 : N_z N_y]$ (as in the Matlab notation system) such that the position indexing is linear as in a 1D array. i as in an index notation, always denotes the field measurement location index and j denotes the source location index. Hence, the 2D spatial Green's function field for a given source location indexed at j is stored as a single column of $G_{ij}^{(0)}$. Thus scanning all possible j locations would result in generating a 2D matrix $G_{ij}^{(0)}$. Within the $[N_y \times N_z]$ grid domain, let there be a disordered slab region spanned by a grid of size $[N_y^P \times N_z^P]$ where the superscript P denotes that it is the grid size referring only to the particle perturbations. In the presence of disorder, the discrete form[35, 36] of Dyson's equation for a 2D transport problem is given as

$$G_{ij} = G_{ij}^{(0)} + \sum_{k=1}^{k=N_z^P N_y^P} G_{ik}^{(0)} V_k \Delta_{area} G_{kj} \quad (1.42)$$

where $V_k = -k_0^2 \delta \tilde{\epsilon}_r(r_k)$ is the scattering potential at the position r_k indexed linearly by $k = 1, 2, 3, \dots, N_z^P N_y^P$ and $\Delta_{area} = \Delta_z \Delta_y$ where $\Delta_z = \Delta_y = \Delta_s$ is the grid size along z and y . Index k is always used to represent positions at which there are disorder perturbations. The equation 1.42 forms a system of equations, in terms of G_{ij} , $G_{ij}^{(0)}$ and the scattering potential. Solving such a system of equations is a computationally expensive process, as there is no approximations²⁶ involved. In [35, 36], an iterative method is provided for updating G_{ij} , starting from $G_{ij}^{(0)}$. Such an iteration method starts from the unperturbed Green's function $G_{ij}^{(0)}$. In the first step, the method updates $G_{ij}^{(0)}$ to $G_{ij}^{(1)}$, where $G_{ij}^{(1)}$ indicates the Green's function due to the scattering perturbation, just at the first scattering grid point. Then, $G_{ij}^{(2)}$ is estimated, bringing in the second scattering grid point and so on, until the final particle is brought in, leading to the evaluation of G_{ij} . In [35, 36], one scattering grid point is taken per iteration, which is computationally tedious to update the

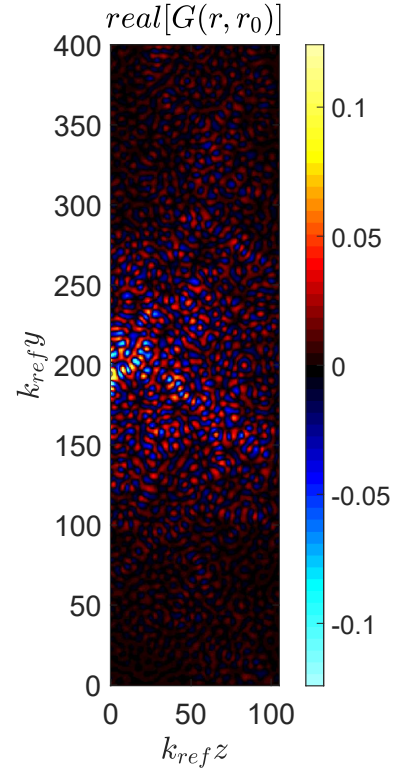


Figure 1.10: The perturbed Green's function $G(z, y, z_0, y_0)$ is shown. The real part of $G(z, y, z_0, y_0)$ is plotted for (z, y) where $(k_{ref} z_0, k_{ref} y_0) = (0, 194.21)$. $G(z, y, z_0, y_0)$ is numerically estimated by following the iterative method given in Section 1.4.2. The random disorder realisation used is given in Figure 1.9.

26: Historically, the Born approximations[40] were first used to analytically simplify the Dyson's equation, taking only the first or the second order of approximation. But, in this chapter, the system of equations given in equation 1.42, is fully solved incorporating all orders of multiple scattering. In other words, in this thesis, there are no approximations involved and the Dyson's equation is solved exactly and fully (like that of [35, 36]), for all the multiple scattering orders.

Green's function matrices, when large number of scattering grid points are involved. Hence, in this chapter, an extension to [35, 36] is proposed, by taking a block of particles together, per iteration step. Description of such a method is provided in the Appendix Section A.8, for better readability of the chapter. In the Appendix Section A.8, two methods are given. First is the direct inversion method (no iteration involved)²⁷, where all the scattering points are taken together, followed by a large matrix inversion. Second method in the Appendix Section A.8 is the proposed iterative method, taking a block of scatterers together, which requires comparatively lesser memory, in comparison with that of the direct method. It is recommended that the reader may go through the direct matrix inversion method first, which is simpler to understand, to obtain a easier grasping of the iterative method. As an example, $G(r, r_0)$ is plotted in Figure 1.10 for a given source location.

27: Such a direct matrix inversion method is memory intensive and it is mainly used for testing the code, for comparing it against the iterative method. The iterative method is the preferred method, which will be used for modelling the results given in this chapter.

1.4.3 Properties of $G_0(r, r_0)$ and $G(r, r_0)$

Some of the properties of the unperturbed Green's function $G_0(r, r_0)$ and the disorder perturbed Green's function $G(r, r_0)$ are provided in this section. These properties will be used later in the chapter for the Kirchhoff–Helmholtz boundary integral formulation of the Helmholtz equation.

Homogeneous boundary conditions for $G_0(r, r_0)$

Any wave (which also includes the Green's function) expanded in terms of eigenmodes $\psi_m^\pm(z, y)$, also satisfy the homogeneous boundary condition for eigenmodes. Hence, the basis expansion components of $G_0(r, r_0)$ also satisfy the homogeneous boundary condition for eigenmodes, similar to that of the equation 1.27, as given below.

Homogeneous boundary conditions for $G_0(r, r_0)$

$$\frac{\partial}{\partial z} G_0^{(m)}(z, z_0, y, y_0)|_{z \geq z_0, (z, y) \in \Gamma_R} - ik_z^{(m)} G_0^{(m)}(z, z_0, y, y_0)|_{z \geq z_0, (z, y) \in \Gamma_R} = 0 \quad (1.43)$$

$$\frac{\partial}{\partial z} G_0^{(m)}(z, z_0, y, y_0)|_{z < z_0, (z, y) \in \Gamma_L} + ik_z^{(m)} G_0^{(m)}(z, z_0, y, y_0)|_{z < z_0, (z, y) \in \Gamma_L} = 0 \quad (1.44)$$

where $G_0^{(m)}(z, z_0, y, y_0)$ is given in equation 1.39.

28: Reciprocity implies that one can exchange the source (r_0) and the field (r) locations, in presence of disorder and obtain the same value for G . For proof in 1D, refer chapter 1.6.3.2 of [41] which is provided for a different context of using ultrasound. For contextualising the proof for a 2D problem with the relevant boundary conditions presented in this chapter, first refer the appendix Section A.9. After that, refer the appendix Section A.10, which explains the reciprocity relationship using the appendix Section A.9.

[41]: Kim et al. (2013), *Sound visualization and manipulation*

Reciprocity of the perturbed Green's function $G(r, r_0)$

Both the unperturbed and the perturbed Green's functions have the property of reciprocity.²⁸ Therefore, $G(r, r_0) = G(r_0, r)$.

Homogeneous boundary conditions for $G(r, r_0)$

The perturbed Green's function $G(r, r_0)$ can also be expanded in terms of the propagating and evanescent eigenmodes $\psi_m^\pm(r)$, which forms a complete basis set. On the left boundary, $G(r, r_0)$ can be expanded in terms of the left going eigenmodes and on the right boundary, $G(r, r_0)$ can be expanded in terms of the right going eigenmodes as given below.

Perturbed Green's function $G(r, r_0)$ in terms of eigenmodes

$$\begin{aligned}
 G(r, r_0)|_{z < z_0, (z, y) \in \Gamma_L} &= \sum_{m=1}^{\infty} G_m(z, y, z_0, y_0)|_{z < z_0, (z, y) \in \Gamma_L} \\
 &= \sum_{m=1}^{\infty} \underbrace{g_m^-(z_0, y_0) \psi_m^-(z, y)}_{G_m(z, y, z_0, y_0)|_{z < z_0, (z, y) \in \Gamma_L}}|_{z < z_0, (z, y) \in \Gamma_L} \quad (1.45)
 \end{aligned}$$

$$\begin{aligned}
 G(r, r_0)|_{z \geq z_0, (z, y) \in \Gamma_R} &= \sum_{m=1}^{\infty} G_m(z, y, z_0, y_0)|_{z \geq z_0, (z, y) \in \Gamma_R} \\
 &= \sum_{m=1}^{\infty} \underbrace{g_m^+(z_0, y_0) \psi_m^+(z, y)}_{G_m(z, y, z_0, y_0)|_{z \geq z_0, (z, y) \in \Gamma_R}}|_{z \geq z_0, (z, y) \in \Gamma_R} \quad (1.46)
 \end{aligned}$$

As the disorder perturbation doesn't change the boundary conditions of the eigenmodes associated with the outgoing Green's function waves, following homogeneous boundary condition can be formed in terms of $G_m(z, y, z_0, y_0)$, similar to that of equations 1.27, 1.43 and 1.44.

Homogeneous boundary conditions for the perturbed Green's function $G(r, r_0)$

$$\frac{\partial}{\partial z} G_m(z, y, z_0, y_0)|_{z < z_0, (z, y) \in \Gamma_L} + i k_z^{(m)} G_m(z, y, z_0, y_0)|_{z < z_0, (z, y) \in \Gamma_L} = 0 \quad (1.47)$$

$$\frac{\partial}{\partial z} G_m(z, y, z_0, y_0)|_{z \geq z_0, (z, y) \in \Gamma_R} - i k_z^{(m)} G_m(z, y, z_0, y_0)|_{z \geq z_0, (z, y) \in \Gamma_R} = 0 \quad (1.48)$$

As of now, the discussions regarding the eigenmodes, $G_0(r, r_0)$ and $G(r, r_0)$, are complete. Next section deals with the estimation of the generalised scattering matrix (S matrix incorporating the propagating and the evanescent modes) from the perturbed Green's function $G(r, r_0)$. The analytical estimation is presented as the following and the discrete formulation follows a similar logic.

1.5 Estimation of the generalised Scattering Matrix from $G(r, r_0)$

The estimation of the generalised scattering matrix of the disorder from the perturbed Green's function $G(r, r_0)$ is explained in the following subsections. The first section gives the Kirchhoff–Helmholtz boundary integral formulation for the total wave estimated using the Helmholtz equation. This is followed by the application of the boundary conditions associated with the boundary integral to simplify the general formulation. Finally, the last section estimates the complex transmission and reflection coefficients of the wave scattering in terms of the transmitted and the

reflected eigenmodes, by matching the total field at the boundaries. First, the evaluation of S_{21} and S_{11} components of the generalised S matrix, where the incident wave is on the left side of the disorder, is explained. Then, the same logic is applied for evaluating the S_{12} and S_{22} part of the generalised S matrix, where the incident wave is on the right side of the disorder.

1.5.1 Kirchhoff–Helmholtz boundary integral formulation

The relation between the Kirchhoff–Helmholtz boundary integral formulation and the conventional Fisher–Lee relations was given by [23], in the context of quantum particle scattering. In the following section, such a relationship is generalised to include the evanescent modes in addition to the propagating modes. First, the goal is to establish the relationship between the perturbed Green's function $G(z, y, z_0, y_0)$ and the total wave field $\tilde{E}(z, y)$ existing inside and around a medium, due to an arbitrary wave incident on the disorder. This helps to estimate the wave scattering response of the disordered medium excited using an arbitrary incident wave. First, let the case of the wave incidence on the sample from the left side be considered, where $\tilde{E}^{inc}(z, y)$ (travelling from left to right) is the incident wave, as shown in the Figure 1.11. On the left boundary Γ_L , the total wave is given as $\tilde{E}(z, y)|_{(z,y) \in \Gamma_L} = \tilde{E}^{inc}(z, y)|_{(z,y) \in \Gamma_L} + \tilde{E}^{refl}(z, y)|_{(z,y) \in \Gamma_L}$ such that $\tilde{E}^{refl}(z, y)|_{(z,y) \in \Gamma_L}$ is the reflected wave onto Γ_L . On the right boundary Γ_R , only the transmitted wave $\tilde{E}^{trans}(z, y)|_{(z,y) \in \Gamma_R}$ exists, therefore the total field $\tilde{E}(z, y)|_{(z,y) \in \Gamma_R} = \tilde{E}^{trans}(z, y)|_{(z,y) \in \Gamma_R}$. Inside the medium, the total field of the wave is denoted as $\tilde{E}(z, y)$ itself. Consider the random media Green's function equation (given in equation 1.31) and also the source free Helmholtz equation (given in equation 1.1)

$$[\nabla^2 + k_0^2 \tilde{\epsilon}_r(z, y)]G(z, y, z_0, y_0) = \delta(z, z_0)\delta(y, y_0), \quad (1.49)$$

$$[\nabla^2 + k_0^2 \tilde{\epsilon}_r(z, y)]\tilde{E}(z, y) = 0, \quad (1.50)$$

where ∇^2 is the Laplacian operator with respect to the field position (z, y) . In the equation 1.49, (z_0, y_0) is the Dirac-delta source location. Multiplying the equation 1.49 using $\tilde{E}(z, y)$ and the equation 1.50 using $G(z, y, z_0, y_0)$, followed by subtraction yields the following

$$\tilde{E}(z, y)[\nabla^2 + k_0^2 \tilde{\epsilon}_r(z, y)]G(z, y, z_0, y_0) = \tilde{E}(z, y)\delta(z, z_0)\delta(y, y_0) \quad (1.51)$$

$$G(z, y, z_0, y_0)[\nabla^2 + k_0^2 \tilde{\epsilon}_r(z, y)]\tilde{E}(z, y) = 0 \quad (1.52)$$

$$\begin{aligned} \textcircled{1.51} - \textcircled{1.52} &= \tilde{E}(z, y)\nabla^2 G(z, y, z_0, y_0) - G(z, y, z_0, y_0)\nabla^2 \tilde{E}(z, y) \\ &= \tilde{E}(z, y)\delta(z - z_0)\delta(y - y_0) \end{aligned} \quad (1.53)$$

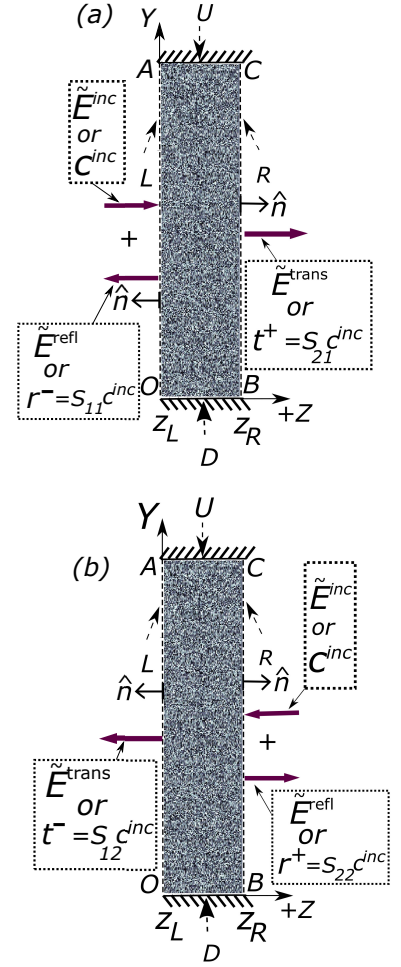


Figure 1.11: The geometry used for estimating the generalised S matrix is shown. This involves the Kirchhoff–Helmholtz boundary integral formulation of the scattering problem. (a) For estimating S_{21} and S_{11} , the wave incidence is from the left side of the disorder. (b) For estimating S_{22} and S_{12} , the wave incidence is from the right side of the disorder. For the wave incidence from left or right side, the YZ coordinate system remains the same. $\tilde{E}^{inc}$ is the incident wave. $\tilde{C}^{inc}$ is a column vector, containing all the complex coefficients used to represent the incident wave $\tilde{E}^{inc}$ as a basis expansion, as given in equation 1.60. Similarly, $\tilde{t}$ and $\tilde{r}$ are column vectors containing coefficients for the transmitted wave and the reflected wave modes, as given in equations 1.62 and 1.72, respectively. + and – as superscripts for $\tilde{r}$ and $\tilde{t}$ denotes the propagation direction (+ implies + z direction and – denotes – z direction) for the reflected and the transmitted waves, respectively. The region enclosed by A, O, B, C is denoted as Ω .

Now integrating in the region Ω enclosed by $AOBCA$, with respect to the field point z and y ,

$$\begin{aligned} & \int \int \left\{ \tilde{E}(z, y) \nabla^2 G(z, y, z_0, y_0) - G(z, y, z_0, y_0) \nabla^2 \tilde{E}(z, y) \right\} dz dy \\ &= \int_{\Omega} \tilde{E}(z, y) \delta(z - z_0) \delta(y - y_0) dz dy = \begin{cases} \tilde{E}(z_0, y_0), & \text{if } (z_0, y_0) \in \Omega \\ 0, & \text{if } (z_0, y_0) \notin \Omega \end{cases} \end{aligned} \quad (1.54)$$

Particularly, the case of $(z_0, y_0) \in \Omega$ is the main interest for the rest of the chapter for evaluating the total field at a desired location $(z_0, y_0) \in \Omega$.²⁹ Using a vector calculus identity³⁰, expression on the L.H.S of equation 1.54 can be re-written as

$$\begin{aligned} & \tilde{E}(z, y) \nabla^2 G(z, y, z_0, y_0) - G(z, y, z_0, y_0) \nabla^2 \tilde{E}(z, y) = \\ & \nabla \cdot \left\{ \tilde{E}(z, y) \nabla G(z, y, z_0, y_0) - G(z, y, z_0, y_0) \nabla \tilde{E}(z, y) \right\} \end{aligned} \quad (1.55)$$

Substituting the above equation back in equation 1.54 and with the help of 2D divergence theorem³¹, the following is obtained.

$$\begin{aligned} & \int \int \nabla \cdot \left\{ \tilde{E}(z, y) \nabla G(z, y, z_0, y_0) - G(z, y, z_0, y_0) \nabla \tilde{E}(z, y) \right\} dz dy \\ &= \int_{\Gamma} \left\{ \tilde{E}(r) \nabla_r G(r, r_0) - G(r, r_0) \nabla_r \tilde{E}(r) \right\} \cdot \hat{n} d\Gamma = \tilde{E}(z_0, y_0) |_{(z_0, y_0) \in \Omega} \end{aligned} \quad (1.56)$$

As there is no flux crossing Γ_U and Γ_D , the above given boundary integral involves only the terms containing Γ_L and Γ_R . The boundary integral can then be simplified³² as

2D Boundary integral formulation of the wave scattering problem

$$\begin{aligned} & \int \left\{ \tilde{E}(z, y) \frac{\partial}{\partial z} G(z, y, z_0, y_0) \hat{e}_z - G(z, y, z_0, y_0) \frac{\partial}{\partial z} \tilde{E}(z, y) \hat{e}_z \right\} |_{(z, y) \in \Gamma_L} \cdot (-\hat{e}_z) dy + \\ & \int \left\{ \tilde{E}(z, y) \frac{\partial}{\partial z} G(z, y, z_0, y_0) \hat{e}_z - G(z, y, z_0, y_0) \frac{\partial}{\partial z} \tilde{E}(z, y) \hat{e}_z \right\} |_{(z, y) \in \Gamma_R} \cdot \hat{e}_z dy = \tilde{E}(z_0, y_0) |_{(z_0, y_0) \in \Omega} \end{aligned} \quad (1.57)$$

The Kirchhoff–Helmholtz boundary integral equation implies that the total field $\tilde{E}(z_0, y_0)$ at a point (z_0, y_0) inside the closed region Ω can be estimated upon knowing the following entities, just at the boundaries.

1) The value of the total field $\tilde{E}(z, y) |_{(z, y) \in \Gamma}$ 2) the Green's function $G(z, y, z_0, y_0)$ and 3) the spatial derivatives of $\tilde{E}(z, y)$ and $G(z, y, z_0, y_0)$ just at the boundaries Γ_L and Γ_R .

The Kirchhoff–Helmholtz boundary integral equation 1.57 can be further simplified, as both $G(z, z, y, y_0)$ and the total field $\tilde{E}(z, y, z_0, y_0) |_{(z, y) \in \Gamma_{L/R}}$ can be expanded in terms of eigenmodes $\psi_m^{\pm}(z, y) |_{(z, y) \in \Gamma_{L/R}}$, followed by the use of the boundary conditions defined before, in equations 1.27, 1.47 and 1.48. As the $E(z, y)$ in equation 1.57 is the total field, the first step to simplify is to provide explicit expression for $\tilde{E}(z, y)$ close to the

31: By the 2D divergence theorem, the integral of the divergence of a vector field in a region Ω , can be replaced by a boundary integral along the boundary Γ , evaluating the flux of the vector field crossing Γ outwards along the surface normal $\hat{n}$ (as shown in Figure 1.11). The integral of the equation 1.55 is also referred to as the Green's second identity. The surface normal $\hat{n}$ points outwards from the surface Γ . Due to the reflection (mirror) boundary condition, there is no flux terms crossing the transverse boundaries Γ_U and Γ_D . Hence, all the spatial derivatives associated with the boundary integral connecting Γ_U and Γ_D , can be safely set to zero.

29: From here (from equation 1.54) to the rest of the chapter, the physical meaning of (z_0, y_0) changes within the context of the Kirchhoff–Helmholtz boundary integral formulation and the Fisher–Lee relations. From here, (z_0, y_0) is not the source location anymore, but the point where the field is evaluated. Such a notion is consistent because of the reciprocity (Refer sec.1.4.3 for the derivation that $G(r, r_0) = G(r_0, r)$) of the Green's function, where one can safely exchange the source position r_0 with field evaluation position r . To prevent ambiguity, it will be explicitly defined in the main equations for the rest of the chapter, where does (z_0, y_0) and (z, y) lie in.

30: The used vector calculus identity is $\nabla \cdot (\phi \nabla \psi) - \nabla \cdot (\psi \nabla \phi) = \phi \nabla^2 \psi - \psi \nabla^2 \phi$ where ψ and ϕ are scalar fields

32: There is a minus sign associated with the $-\hat{e}_z dy$ on the first integral of the L.H.S in equation 1.57. This is due to the sign convention that the surface normal $\hat{n}$ points outwards on Γ_L which is in opposite direction to $\hat{e}_z \frac{\partial}{\partial z}$ terms.

boundary Γ_L and Γ_R , followed by the use of the boundary conditions involving the z derivatives of $\tilde{E}(z, y)$ and $G(z, y, z_0, y_0)$, to be explained in the following section.

1.5.2 Boundary conditions for simplifying the boundary integral equation

For simplifying the equation 1.57, the eigenmode expansions for the incident wave field $\tilde{E}^{inc}(z, y)|_{(z,y) \in \Gamma_L}$, the reflected wave field $\tilde{E}^{refl}(z, y)|_{(z,y) \in \Gamma_L}$ and the transmitted wave field $\tilde{E}^{trans}(z, y)|_{(z,y) \in \Gamma_R}$ need to be defined, which involves the definition³³ of the scattering matrix S in the following block matrix form.

$$S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \quad (1.58)$$

Here, S_{11} and S_{21} are submatrices representing the complex reflection and transmission coefficients associated with the wave incidence on the left side of the disorder. Similarly, S_{22} and S_{12} are submatrices representing the complex reflection and transmission coefficients associated with the wave incidence on the right side of the disorder. In this chapter, the conventional definition of S matrix is generalised to include the evanescent modes as well, in addition to the propagating modes. For the dimensions of the submatrices contained in the S matrix, refer the sidenote.³⁴ First, let the scenario of the wave incidence from the left side of the disorder be considered, which involves the S_{21} and S_{11} part of the S matrix. On Γ_L , there are right going wave (incident wave $\tilde{E}^{inc}(z, y)|_{(z,y) \in \Gamma_L}$) and left going waves (reflected wave, $\tilde{E}^{refl}(z, y)|_{(z,y) \in \Gamma_L}$). Hence, the total wave field $\tilde{E}(z, y)|_{(z,y) \in \Gamma_L}$ is written as the following.

Total field on Γ_L due to wave incidence from left onto Γ_L

$$\tilde{E}(z, y)|_{(z,y) \in \Gamma_L} = \tilde{E}^{inc}(z, y)|_{(z,y) \in \Gamma_L} + \tilde{E}^{refl}(z, y)|_{(z,y) \in \Gamma_L} \quad (1.59)$$

$$\begin{aligned} \tilde{E}^{inc}(z, y)|_{(z,y) \in \Gamma_L} &= \sum_{m=1}^{M_{total}} c_m^+ \chi_m(y) \phi_m^+(z) \\ \text{where } \phi_m^+(z) &= \begin{cases} \phi_{m,prop}^+(z) & \text{when } m \leq M_{prop} \\ \phi_{m,evan}^+(z, z_L) & \text{when } m > M_{prop} \end{cases} \end{aligned} \quad (1.60)$$

$$\tilde{E}^{refl}(z, y)|_{(z,y) \in \Gamma_L} = \sum_{n=1}^{N_{total}} r_n^- \chi_n(y) \phi_n^-(z) \quad (1.61)$$

$$\text{where } \phi_n^-(z) = \begin{cases} \phi_{n,prop}^-(z) & \text{when } n \leq N_{prop} \\ \phi_{n,evan}^-(z, z_L) & \text{when } n > N_{prop} \end{cases}$$

and r_n^- is the reflection³⁵ coefficient given as

$$r_n^- = \sum_{m=1}^{M_{total}} S_{11}^{nm} c_m^+ \quad (1.62)$$

33: For the conventional definition of scattering matrix, refer section II.A.4 of [18], followed by the schematics given in Figure 1.11.

34: The dimension of the transmission matrix S_{21} is generally given as $[N_{total} \times M_{total}]$ where M_{total} is the number of incident eigenmodes and N_{total} the number of transmitted eigenmodes. $M_{total} = M_{prop} + M_{evan}$. Here, M_{prop} is the total number of propagating eigenmodes. M_{evan} is the number of evanescent modes taken numerically which is a truncation number as said before. Similarly, $N_{total} = N_{prop} + N_{evan}$. For the quasi-1D transport problem defined in the chapter, $M_{total} = N_{total}$. For the reflection matrix S_{11} , the dimension is given as $[M_{total} \times M_{total}]$. Similarly, the dimensions of the S_{12} and S_{22} can be defined.

35: r_n^- is the field reflection coefficient term associated with the n^{th} reflected eigenmode and c_m^+ is the coefficient for the right going incident eigenmode, where S_{11}^{nm} denotes the n^{th} row & m^{th} column element of the reflection matrix.

Substituting the equations 1.60 and 1.61 in 1.59, and using a property³⁶ of the Kronecker delta function, the following is obtained.

$$\begin{aligned} \tilde{E}(z, y)|_{(z, y) \in \Gamma_L} = & \sum_{n=1}^{N_{total}} \sum_{m=1}^{M_{total}} c_m^+ \phi_m^+(z) \chi_m(y) \delta_{kron}(n, m)|_{(z, y) \in \Gamma_L} + \\ & \sum_{n=1}^{N_{total}} \sum_{m=1}^{M_{total}} c_m^+ S_{11}^{nm} \chi_n(y) \phi_n^-(z)|_{(z, y) \in \Gamma_L} \end{aligned} \quad (1.63)$$

Due to the Kronecker delta on the first term on the R.H.S of the above given equation, the index m can be replaced by n to obtain³⁷

$$\begin{aligned} \tilde{E}(z, y)|_{(z, y) \in \Gamma_L} = & \sum_{n=1}^{N_{total}} \sum_{m=1}^{M_{total}} c_m^+ \left\{ \phi_n^+(z) \chi_n(y) \delta_{kron}(n, m) + S_{11}^{nm} \chi_n(y) \phi_n^-(z) \right\} |_{(z, y) \in \Gamma_L} \\ & \underbrace{\tilde{E}_n(z, y)|_{(z, y) \in \Gamma_L}} \end{aligned} \quad (1.64)$$

$$= \sum_{n=1}^{N_{total}} \tilde{E}_n(z, y)|_{(z, y) \in \Gamma_L} \quad (1.65)$$

Equation 1.64 denotes that the total field on Γ_L can be written as a series summation involving $\tilde{E}_n(z, y)|_{(z, y) \in \Gamma_L}$ waves. Next, the boundary condition associated with $\tilde{E}_n(z, y)|_{(z, y) \in \Gamma_L}$ waves, for simplifying the boundary integral equation, is provided. For the proof, refer to the side note.³⁸

Inhomogeneous boundary condition on Γ_L for $\tilde{E}_n$

$$\begin{aligned} & \frac{\partial}{\partial z} \tilde{E}_n(z, y)|_{(z, y) \in \Gamma_L} + i k_z^{(n)} \tilde{E}_n(z, y)|_{(z, y) \in \Gamma_L} \\ & = \begin{cases} 2i k_z^{(n)} \tilde{E}_n^{inc}(z, y)|_{(z, y) \in \Gamma_L}, & \text{if } 1 \leq n \leq M_{total} \\ 0, & \text{if } n > M_{total} \end{cases} \end{aligned} \quad (1.70)$$

which is the inhomogeneous³⁹ boundary condition, where $\tilde{E}_n^{inc}(z, y)|_{(z, y) \in \Gamma_L} = c_n^+ \psi_n^+(z, y)|_{(z, y) \in \Gamma_L}$ is the n^{th} eigenmode term associated with the incident wave, incident on the disorder from the left and $k_z^{(n)} = i k_{z, evan}^{(n)}$ for the evanescent modes.

Next is to evaluate the transmitted total field on Γ_R , due to the wave incidence from left side upon Γ_L and the associated boundary condition.

36: The Kronecker delta function has a property that $\sum_n f_n \delta_{kron}(n, m) = f_m$.

37: The total wave $\tilde{E}(z, y)|_{(z, y) \in \Gamma_L}$ is written as a summation of $\tilde{E}_n(z, y)|_{(z, y) \in \Gamma_L}$ modes. The boundary conditions for $\tilde{E}(z, y)|_{(z, y) \in \Gamma_L}$ is equivalent to the estimation of the boundary conditions for $\tilde{E}_n(z, y)|_{(z, y) \in \Gamma_L}$ modes.

38: Taking the partial derivative of equation 1.64,

$$\begin{aligned} & \frac{\partial}{\partial z} E_n(z, y)|_{(z, y) \in \Gamma_L} = \\ & \sum_{m=1}^{M_{total}} c_m^+ [\delta_{kron}(n, m) \frac{\partial}{\partial z} \psi_n^+(z, y) + \\ & S_{11}^{nm} \frac{\partial}{\partial z} \psi_n^-(z, y)] \end{aligned} \quad (1.66)$$

Using equation 1.27,

$$\begin{aligned} & \frac{\partial}{\partial z} E_n(z, y)|_{(z, y) \in \Gamma_L} = \\ & \sum_{m=1}^{M_{total}} c_m^+ [\delta_{kron}(n, m) \{ i k_z^{(n)} \psi_n^+(z, y) \} + \\ & S_{11}^{nm} \{ -i k_z^{(n)} \psi_n^-(z, y) \}] \\ & = \sum_{m=1}^{M_{total}} i k_z^{(n)} c_m^+ [\delta_{kron}(n, m) \psi_n^+(z, y) \\ & - S_{11}^{nm} \psi_n^-(z, y)] \end{aligned} \quad (1.67)$$

Using equation 1.64 once again,

$$\begin{aligned} & i k_z^{(n)} E_n(z, y)|_{(z, y) \in \Gamma_L} = \\ & \sum_{m=1}^{M_{total}} i k_z^{(n)} c_m^+ [\delta_{kron}(n, m) \psi_n^+(z, y) + \\ & S_{11}^{nm} \psi_n^-(z, y)] \end{aligned} \quad (1.68)$$

Therefore, adding the equations together,

$$\begin{aligned} & \frac{\partial}{\partial z} E_n(z, y)|_{(z, y) \in \Gamma_L} + i k_z^{(n)} E_n(z, y)|_{(z, y) \in \Gamma_L} = \\ & \sum_{m=1}^{M_{total}} 2i k_z^{(n)} c_m^+ [\delta_{kron}(n, m) \psi_n^+(z, y)] \end{aligned} \quad (1.69)$$

Due to the Kronecker delta function, the summation in the RHS fires up only when $m = n$, hence the boundary condition given in 1.70 is obtained.

39: One may note that on the R.H.S of equation 1.70 contains the incident wave, making it an inhomogeneous boundary condition on the left boundary Γ_L .

Total field on Γ_R due to the wave incidence from the left onto Γ_L

$$\tilde{E}(z, y)|_{(z,y) \in \Gamma_R} = \tilde{E}^{trans}(z, y)|_{(z,y) \in \Gamma_R} = \sum_{n=1}^{N_{total}} t_n^+ \phi_n^+(z) \chi_n(y)|_{(z,y) \in \Gamma_R}$$

$$\text{where } \phi_n^+(z) = \begin{cases} \phi_{n,prop}^+(z) & \text{when } n \leq N_{prop} \\ \phi_{n,evan}^+(z, z_R) & \text{when } n > N_{prop} \end{cases} \quad (1.71)$$

where the field transmission coefficient term t_n^+ is related to the transmission matrix S_{21} by

$$t_n^+ = \sum_{m=1}^{M_{total}} S_{21}^{nm} c_m^+ \quad (1.72)$$

Therefore,

$$\tilde{E}(z, y)|_{(z,y) \in \Gamma_R} = \sum_{n=1}^{N_{total}} \underbrace{\left\{ \sum_{m=1}^{M_{total}} c_m^+ S_{21}^{nm} \right\}}_{\tilde{E}_n(z, y)|_{(z,y) \in \Gamma_R}} \phi_n^+(z) \chi_n(y)|_{(z,y) \in \Gamma_R} \quad (1.73)$$

$$= \sum_{n=1}^{N_{total}} \tilde{E}_n(z, y)|_{(z,y) \in \Gamma_R} \quad (1.74)$$

Similar to that of equation 1.70, one could form a boundary condition for $E_n(z, y)|_{(z,y) \in \Gamma_R}$ on the right boundary Γ_R as given below, to be used to simplify the boundary integral equation given in 1.57. This homogeneous boundary condition can be easily verified using equations 1.73 and 1.74.

Homogeneous boundary condition on Γ_R for $\tilde{E}_n$

$$\frac{\partial}{\partial z} \tilde{E}_n(z, y)|_{(z,y) \in \Gamma_R} - ik_z^{(n)} \tilde{E}_n(z, y)|_{(z,y) \in \Gamma_R} = 0 \quad (1.75)$$

The next section explains the simplification of the boundary integral given in equation 1.57, involving the homogeneous and the inhomogeneous boundary conditions associated with $G_m(z, z_0, y, y_0)$ and $\tilde{E}_n(z, y)$, at Γ_L and Γ_R .

1.5.3 Simplified boundary integral equation for the total field estimation

A key aspect of simplifying the equation 1.57, is to substitute the basis expansion for $G(z, z_0, y, y_0) = \sum_{m=1}^{M_{total}} G_m(z, y, z_0, y_0)$ and $\tilde{E}(z, y)|_{(z,y) \in \Gamma_{L/R}} = \sum_{n=1}^{N_{total}} \tilde{E}_n(z, y)|_{(z,y) \in \Gamma_{L/R}}$ and their corresponding boundary conditions.

The equation 1.57 is then written as

$$\begin{aligned} & \int \left\{ \sum_n \tilde{E}_n(z, y) \frac{\partial}{\partial z} \sum_m G_m(z, y, z_0, y_0) \hat{e}_z - \sum_m G_m(z, y, z_0, y_0) \frac{\partial}{\partial z} \sum_n \tilde{E}_n(z, y) \hat{e}_z \right\} |_{(z,y) \in \Gamma_L} \cdot (-\hat{e}_z) dy + \\ & \int \left\{ \sum_n \tilde{E}_n(z, y) \frac{\partial}{\partial z} \sum_m G_m(z, y, z_0, y_0) \hat{e}_z - \sum_m G_m(z, y, z_0, y_0) \frac{\partial}{\partial z} \sum_n \tilde{E}_n(z, y) \hat{e}_z \right\} |_{(z,y) \in \Gamma_R} \cdot \hat{e}_z dy \\ & = \tilde{E}(z_0, y_0) |_{(z_0, y_0) \in \Omega} \end{aligned} \quad (1.76)$$

As there is a $\chi_m(y)$ in $G_m(z, y, z_0, y_0)$ and due to the $\chi_n(y)$ in $\tilde{E}_n(z, y)$, by the orthogonality relation that $\int \chi_m(y) \chi_n(y) dy = \delta_{kron}(m, n)$, the y integral of all the cross product terms where $m \neq n$, is zero. Hence, only the terms $m = n$ remains non-zero. Therefore,

$$\begin{aligned} & \int \sum_n \left\{ \tilde{E}_n(z, y) \frac{\partial}{\partial z} G_n(z, y, z_0, y_0) \hat{e}_z - G_n(z, y, z_0, y_0) \frac{\partial}{\partial z} \tilde{E}_n(z, y) \hat{e}_z \right\} |_{(z,y) \in \Gamma_L} \cdot (-\hat{e}_z) dy + \\ & \int \sum_n \left\{ \tilde{E}_n(z, y) \frac{\partial}{\partial z} G_n(z, y, z_0, y_0) \hat{e}_z - G_n(z, y, z_0, y_0) \frac{\partial}{\partial z} \tilde{E}_n(z, y) \hat{e}_z \right\} |_{(z,y) \in \Gamma_R} \cdot \hat{e}_z dy \\ & = \tilde{E}(z_0, y_0) |_{(z_0, y_0) \in \Omega} \end{aligned} \quad (1.77)$$

Substituting the previously obtained boundary conditions (equations 1.48, 1.75, 1.47 and 1.70) in the above given boundary integral, the following simplified expression is obtained, after some simple calculations.⁴⁰

$$\int \sum_n 2ik_z^{(n)} \tilde{E}_n^{inc}(z, y) G_n(z, y, z_0, y_0) |_{(z,y) \in \Gamma_L} dy = \tilde{E}(z_0, y_0) |_{(z_0, y_0) \in \Omega} \quad (1.79)$$

One could safely add a summation $\sum_m$ to the $G_m(z, y, z_0, y_0)$ term in the above equation, due to the orthogonality relationship $\int \chi_m(y) \chi_n(y) dy = \delta_{kron}(m, n)$. Therefore, the meaning of the integral given in 1.79 doesn't change⁴¹, if it is written in the following form.

$$\int \sum_n 2ik_z^{(n)} \tilde{E}_n^{inc}(z, y) \sum_m G_m(z, y, z_0, y_0) |_{(z,y) \in \Gamma_L} dy = \tilde{E}(z_0, y_0) |_{(z_0, y_0) \in \Omega} \quad (1.80)$$

Replacing the expression for $\sum_m G_m(z, y, z_0, y_0)$ as $G(z, y, z_0, y_0)$ and changing the index n to m , the boundary integral takes a simpler form as given below.

Simplified boundary integral formulation for the wave incidence onto the left side of the disorder (incidence onto Γ_L)

$$\sum_{m=1}^{M_{total}} 2ik_z^{(m)} \int \tilde{E}_m^{inc}(z, y) G(z, y, z_0, y_0) |_{(z,y) \in \Gamma_L} dy = \tilde{E}(z_0, y_0) |_{(z_0, y_0) \in \Omega} \quad (1.81)$$

where $\tilde{E}_m^{inc}(z, y) |_{(z,y) \in \Gamma_L} = c_m^+ \psi_m^+(z, y) |_{(z,y) \in \Gamma_L}$ and $k_z^{(m)} = ik_{z,even}^{(m)}$ when $m > M_{prop}$

40: The expressions used for simplifying the equation 1.77, is summarised as the following: The terms in the second curly brace {...} in the equation 1.77 cancels off each other to zero because for $(z, y) \in \Gamma_R$, (using equations 1.48 and 1.75),

$$\begin{aligned} & \frac{\partial}{\partial z} G_n(z, y, z_0, y_0) |_{(z,y) \in \Gamma_R} = \\ & ik_z^{(n)} G_n(z, y, z_0, y_0) |_{(z,y) \in \Gamma_R} \end{aligned}$$

$$\frac{\partial}{\partial z} E_n(z, y) |_{(z,y) \in \Gamma_R} = ik_z^{(n)} E_n(z, y) |_{(z,y) \in \Gamma_R}$$

Most of the terms in the first curly brace {...} in the equation 1.77 cancels off each other, except for the inhomogeneous incident wave term which remains (using equations 1.47 and 1.70)

$$\begin{aligned} & \frac{\partial}{\partial z} G_m(z, y, z_0, y_0) = \\ & -ik_z^{(m)} G_m(z, y, z_0, y_0) |_{(z,y) \in \Gamma_L} \\ & \frac{\partial}{\partial z} E_n(z, y) = 2ik_z^{(n)} \tilde{E}_n^{inc}(z, y) |_{(z,y) \in \Gamma_L} \\ & -ik_z^{(n)} E_n(z, y) |_{(z,y) \in \Gamma_L} \end{aligned} \quad (1.78)$$

41: Such a reformulation is justified because there is a $\chi_m(y)$ in $G_m(z, y, z_0, y_0)$ and a $\chi_n(y)$ in $\tilde{E}_n^{inc}(z, y)$. Due to the orthogonality relation $\int \chi_m(y) \chi_n(y) dy = \delta_{kron}(m, n)$, y integral of all the cross product terms where $m \neq n$, is zero. Hence only the terms $m = n$ remains non-zero, recovering the integral given in equation 1.79.

The above given boundary integral will be used for the visualisation of

the total field⁴² and also to evaluate the S_{21} and S_{11} components of the S matrix, when the wave incidence is from the left side of the disorder. For estimating S_{22} and S_{12} components of the S matrix, where the wave is incident from the right side of the disorder onto Γ_R , the simplified boundary integral equation for the wave incidence from the right, has to be defined as the following. In such a case, the equation gets modified as

Simplified boundary integral formulation for the wave incidence onto the right side of the disorder (incidence onto Γ_R)

$$\sum_{m=1}^{M_{total}} 2ik_z^{(m)} \int \tilde{E}_m^{inc}(z, y) G(z, y, z_0, y_0) |_{(z,y) \in \Gamma_R} dy = \tilde{E}(z_0, y_0) |_{(z_0, y_0) \in \Omega} \quad (1.82)$$

where $\tilde{E}_m^{inc}(z, y) |_{(z,y) \in \Gamma_R} = c_m^- \psi_m^-(z, y) |_{(z,y) \in \Gamma_R}$ and $k_z^{(m)} = ik_{z, evan}^{(m)}$ when $m > M_{prop}$.

Next section explains how the reflection and the transmission matrices can be obtained from the boundary integral equation presented in the equation 1.81. The concept for implementing that is based on the Fisher-Lee relations[18, 21, 23, 42] for electronic conductance. In this chapter, the traditional Fisher-Lee method (incorporating only the propagating modes) is generalised to include the evanescent wave modes as well. These evanescent modes are particularly significant in the sub-wavelength light focussing[22] experiments, involving the near-field scanning optical microscopy probes.⁴³ Incorporating the evanescent modes will also enable the cascading of the S matrices, to be discussed in the later part of this chapter. The motivation for implementing the Fisher-Lee relations is for directly estimating the S matrix from the Green's function. Such relationship is derived from the simplified boundary integral equation in the following section.

1.5.4 Generalised Fisher-Lee relation for estimating the generalised S matrix containing evanescent modes

The boundary integral equation (equation 1.81) gives the value of the total field $\tilde{E}(z_0, y_0) |_{(z_0, y_0) \in \Omega}$, for a given incident field $E^{inc}(z, y) |_{(z,y) \in \Gamma_L}$, using the Green's function $G(z, y, z_0, y_0) |_{(z,y) \in \Gamma_L}$ where $(z_0, y_0) \in \Omega$. But, the total field is known on the left boundary $(z_0, y_0) \in \Gamma_L$ (which is still within Ω), as the sum of the incident wave mode and the reflected wave mode, involving the S_{11} matrix. As the total field is continuous across Γ_L , one could estimate S_{11} by matching the total field estimated on Γ_L , using the boundary integral and the definition of the total field on Γ_L , involving S_{11} . Similar analysis can be performed on the total field at the right boundary $(z_0, y_0) \in \Gamma_R$, involving S_{21} . Such an analysis can be related to the conventional Fisher-Lee relation [18, 21, 23, 42]. In this section, generalisation to the conventional Fisher-Lee relation, incorporating the evanescent modes, is discussed. The estimation of S_{11} and S_{21} is discussed first and in the next subsection, estimation of S_{22} and S_{12} is covered.

42: The simplified boundary integral equation will be used throughout in the chapter for visualising the field $\tilde{E}(z_0, y_0)$, where (z_0, y_0) is inside the region Ω , for a given incident wave $\tilde{E}^{inc}(z, y) |_{(z,y) \in \Gamma_L}$. For evaluating the field $\tilde{E}(z_0, y_0)$ at a certain desired location (z_0, y_0) , due to a wave incidence from the left side of the disorder, the perturbed Green's function $G(z, y, z_0, y_0) |_{(z,y) \in \Gamma_L}$ and the incident field at the left boundary $E^{inc}(z, y, z_0, y_0) |_{(z,y) \in \Gamma_L}$, is needed

[21]: Fisher et al. (1981), 'Relation between conductivity and transmission matrix'

[42]: Datta (1997), *Electronic transport in mesoscopic systems*

[23]: Dömötör et al. (2015), 'Scattering of a particle with internal structure from a single slit: exact numerical solutions'

[18]: Rotter et al. (2017), 'Light fields in complex media: Mesoscopic scattering meets wave control'

[22]: Park et al. (2017), 'Time-reversing a monochromatic subwavelength optical focus by optical phase conjugation of multiply-scattered light'

43: [22] used a subwavelength light source (probe tip of a Near-field Scanning Optical Microscope (NSOM)) injecting evanescent modes onto random nanoparticles, which gets scattered as propagating modes in the far field. Such a transmitted propagating wave is phase-conjugated through the disorder to attain sub-wavelength focusing back at the source location.

First, let the wave incidence be from the left to the right of the disorder, for the estimation of S_{11} and S_{21} as given below. The associated proofs are given in Section A.11.1 and Section A.11.2, respectively. For the estimation of S_{11} , $(z = 0, y) \in \Gamma_L$ & $(z_0 = 0, y_0) \in \Gamma_L$. Let there be an integral⁴⁴ defined as the following,

$$G_{nm}^{S_{11}} = \int \int \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) dy dy_0 |_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_L} \quad (1.83)$$

Then, the elements of the matrix S_{11} , in terms of $G_{nm}^{S_{11}}$ are given in the Table 1.1, where the terms under $Inc(m)$ denotes the nature⁴⁵ of the m^{th} incident wave mode and the terms under $Ref(n)$ denotes the nature of the reflected wave mode.

Table 1.1: Matrix elements of S_{11}

$Inc(m)$	$Ref(n)$	S_{11}^{nm}
<i>prop</i>	<i>prop</i>	$-\delta_{kron}(n, m) + 2i\sqrt{k_z^{(m)}}\sqrt{k_z^{(n)}}G_{nm}^{S_{11}}$
<i>evan</i>	<i>evan</i>	$-\delta_{kron}(n, m) + 2\sqrt{ k_z^{(m)} }\sqrt{ k_z^{(n)} }G_{nm}^{S_{11}}$
<i>prop</i>	<i>evan</i>	$2i\sqrt{k_z^{(m)}}\sqrt{ k_z^{(n)} }G_{nm}^{S_{11}}$
<i>evan</i>	<i>prop</i>	$-2\sqrt{ k_z^{(m)} }\sqrt{k_z^{(n)}}G_{nm}^{S_{11}}$

44: The integral can be interpreted as a double-Fourier-like decomposition in the eigenspace, of the Green's function component used for estimating S_{11} .

45: The incident wave modes can either be propagating (*prop*) when $m \leq M_{prop}$ or be evanescent (*evan*) when $m > M_{prop}$. Similarly, the reflected or the transmitted wave modes can also be either propagating (*prop*) when $n \leq N_{prop}$ or be evanescent (*evan*) when $n > N_{prop}$.

For the estimation of S_{21} , $(z = 0, y) \in \Gamma_L$ & $(z_0 = z_R, y_0) \in \Gamma_R$. Let there be an integral defined as

$$G_{nm}^{S_{21}} = \int \int \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) dy dy_0 |_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_R} \quad (1.84)$$

Then, the elements of the matrix S_{21} , in terms of $G_{nm}^{S_{21}}$ are given in the Table 1.2.

Table 1.2: Matrix elements of S_{21}

$Inc(m)$	$Trans(n)$	S_{21}^{nm}
<i>prop</i>	<i>prop</i>	$2i\sqrt{k_z^{(m)}}\sqrt{k_z^{(n)}}e^{-iz_R k_z^{(n)}}G_{nm}^{S_{21}}$
<i>evan</i>	<i>evan</i>	$-2\sqrt{ k_z^{(m)} }\sqrt{ k_z^{(n)} }G_{nm}^{S_{21}}$
<i>prop</i>	<i>evan</i>	$2i\sqrt{k_z^{(m)}}\sqrt{ k_z^{(n)} }G_{nm}^{S_{21}}$
<i>evan</i>	<i>prop</i>	$-2\sqrt{ k_z^{(m)} }\sqrt{k_z^{(n)}}e^{-iz_R k_z^{(n)}}G_{nm}^{S_{21}}$

For evaluating S_{22} and S_{12} , incident wave propagates from right side onto Γ_R . Hence, the total field on Γ_R consists of the superposition of the incident wave and the reflected wave. Total field on Γ_L is the transmitted wave propagating to the left side of the disorder. For the estimation of S_{22} , $(z = z_R, y) \in \Gamma_R$ and $(z_0 = z_R, y_0) \in \Gamma_R$. Let there be an integral

defined

$$G_{nm}^{S_{22}} = \int \int \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) dy dy_0 |_{(z,y) \in \Gamma_R \& (z_0,y_0) \in \Gamma_R} \quad (1.85)$$

Then, the elements of the matrix S_{22} in terms of $G_{nm}^{S_{22}}$ are given in the Table 1.3.

Table 1.3: Matrix elements of S_{22}

$Inc(m)$	$Ref l(n)$	S_{22}^{nm}
<i>prop</i>	<i>prop</i>	$-\delta_{kron}(n, m) e^{-iz_R(k_z^{(m)} + k_z^{(n)})} + 2i\sqrt{k_z^{(n)}}\sqrt{k_z^{(m)}} e^{-iz_R(k_z^{(m)} + k_z^{(n)})} G_{nm}^{S_{22}}$
<i>evan</i>	<i>evan</i>	$-\delta_{kron}(n, m) + -2\sqrt{ k_z^{(m)} }\sqrt{ k_z^{(n)} } G_{nm}^{S_{22}}$
<i>prop</i>	<i>evan</i>	$+2i\sqrt{k_z^{(m)}}\sqrt{ k_z^{(n)} } e^{-iz_R k_z^{(m)}} G_{nm}^{S_{22}}$
<i>evan</i>	<i>prop</i>	$-2\sqrt{ k_z^{(m)} }\sqrt{k_z^{(n)}} e^{-iz_R k_z^{(n)}} G_{nm}^{S_{22}}$

For the evaluation of S_{12} , $(z, y) \in \Gamma_R$ & $(z_0, y_0) \in \Gamma_L$ and define the integral

$$G_{nm}^{S_{12}} = \int \int \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) dy dy_0 |_{(z,y) \in \Gamma_R \& (z_0,y_0) \in \Gamma_L} \quad (1.86)$$

Finally, the elements of the matrix S_{12} in terms of $G_{nm}^{S_{12}}$ are given in the Table 1.4.

Table 1.4: Matrix elements of S_{12}

$Inc(m)$	$Trans(n)$	S_{12}^{nm}
<i>prop</i>	<i>prop</i>	$2i\sqrt{k_z^{(m)}}\sqrt{k_z^{(n)}} e^{-iz_R k_z^{(m)}} G_{nm}^{S_{12}}$
<i>evan</i>	<i>evan</i>	$-2\sqrt{ k_z^{(m)} }\sqrt{ k_z^{(n)} } G_{nm}^{S_{12}}$
<i>prop</i>	<i>evan</i>	$2i\sqrt{k_z^{(m)}}\sqrt{ k_z^{(n)} } e^{-iz_R k_z^{(m)}} G_{nm}^{S_{12}}$
<i>evan</i>	<i>prop</i>	$-2\sqrt{ k_z^{(m)} }\sqrt{k_z^{(n)}} G_{nm}^{S_{12}}$

The tables 1.1, 1.2, 1.3 and 1.4 are the main results proposed in this section. The numerically estimated S matrix using the given tables, is shown in Figure 1.12. Such a generalised S matrix containing evanescent modes, was first described analytically by Carminati et al.[20] and later generalised by Byrnes and Foreman[24]. The next section gives the numerical validation of the generalised reciprocity and unitarity relations, involving the S matrix.

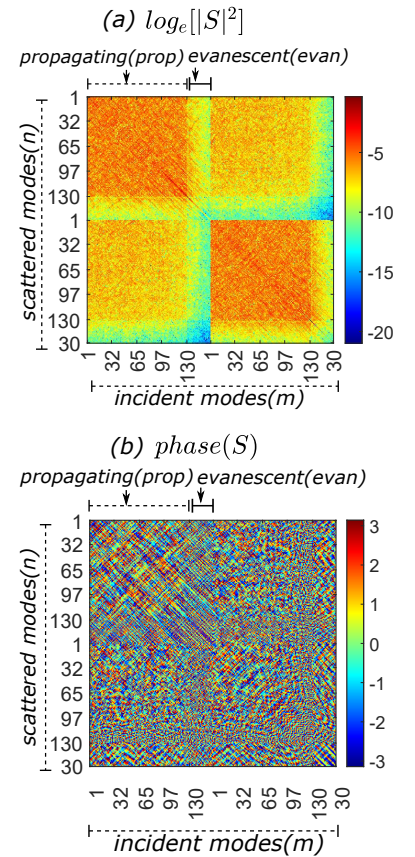


Figure 1.12: An example S matrix estimated using the tables 1.1, 1.2, 1.3 and 1.4, is plotted. (a) Squared magnitude of S matrix (plotted in $\log_e$ scale) given in equation 1.58, estimated using the generalized Fisher-Lee relations given in Tables 1.1, 1.2, 1.3, and 1.4. The disorder shown in Figure 1.9 is used for the quasi-1D geometry (obtained without any S matrix cascading). The number of propagating modes involved for wave incidence and scattering is 130 and the number of evanescent modes is 30. (b) Phase of the S matrix elements is plotted.

1.5.5 Numerical validation of the generalised reciprocity and unitarity relations, involving the evanescent modes

The S matrix estimated in this chapter, has the generalised unitarity property, which is based on the conservation of wave flux. The analytical form of the generalized unitarity relation, for a discrete angular spectrum is provided in [24], where a partitioned S matrix ($S_{\text{partitioned}}$) is defined to compactly evaluate the unitarity relationship. The $S_{\text{partitioned}}$ defined in [24], rearranges the S matrix defined in equation 1.58, to the following form

$$S_{\text{partitioned}} = \begin{bmatrix} S_{\text{partitioned}}^{\text{prop,prop}} & S_{\text{partitioned}}^{\text{prop,evan}} \\ S_{\text{partitioned}}^{\text{evan,prop}} & S_{\text{partitioned}}^{\text{evan,evan}} \end{bmatrix} \quad (1.87)$$

As an example, $S_{\text{partitioned}}^{\text{prop,evan}}$ contains those elements of the S matrix, which have incident modes being evanescent and scattered modes being propagating, grouped together as shown in Figure 1.13(b). Similarly, $S_{\text{partitioned}}^{\text{prop,prop}}$ represents the part of the S matrix, where both the incident modes and the scattered modes, are propagating modes. It could then be inferred that $S_{\text{partitioned}}^{\text{evan,evan}}$ contains both the incident modes and the scattered modes, evanescent. Finally, $S_{\text{partitioned}}^{\text{evan,prop}}$ contains those elements of the S matrix, which have incident modes being propagating and scattered modes being evanescent. A selection mask matrix (of the same size that of the S matrix) used to crop the S matrix, to yield the $S_{\text{partitioned}}$, is given in Figure 1.13(a), where the blue colour denotes unity and the white colour for zero. The selection mask shown in Figure 1.13(a) has four parts, each associated for extracting a certain part of the S matrix. For example, using the $\text{Mask}(\text{prop}, \text{prop})$ for element-wise multiplication with the S matrix shown in Figure 1.12, is used to extract the propagating part (of the size $2N_{\text{prop}} \times 2M_{\text{prop}}$) of the S matrix, where both the incident and the scattered modes are propagating. Similarly, using the mask $\text{Mask}(\text{evan}, \text{prop})$ results in extracting that part of the S matrix (of size $2N_{\text{evan}} \times 2M_{\text{prop}}$), where the incident modes are propagating and the scattered modes are evanescent. Likewise, $\text{Mask}(\text{evan}, \text{evan})$ extracts the purely evanescent part (of size $2N_{\text{evan}} \times 2M_{\text{evan}}$) of the S matrix. Finally, $\text{Mask}(\text{prop}, \text{evan})$ results in extracting that part of the S matrix (of size $2N_{\text{prop}} \times 2M_{\text{evan}}$), where the incident modes are evanescent and the scattered modes are propagating. All the extracted sub-matrices, forms the $S_{\text{partitioned}}$, as shown in the Figure 1.13(b). Such a partitioned S matrix is used to numerically validate (refer Figure 1.14(a)), the unitarity relation, based on the analytical results given by [20, 24], as shown in Figure 1.14. Next, the generalized reciprocity relations are summarised, by comparing the expressions for S_{11} , S_{21} , S_{12} , S_{22} between tables 1.1, 1.2, 1.3 and 1.4, respectively. Comparing the expressions given in the first two rows of all the tables, where m and n are either both propagating or both evanescent, we get $S_{11}^{nm} = S_{11}^{mn}$, $S_{22}^{nm} = S_{22}^{mn}$, and $S_{21}^{nm} = S_{12}^{mn}$. This is due to the perturbed Green's function reciprocity symmetry, such that $G(r, r_0) = G(r_0, r)$, implying $G_{nm} = G_{mn}$. On the other hand, when $m \leq M_{\text{prop}}$ and $n > N_{\text{prop}}$, then $S_{11}^{mn} = iS_{11}^{nm}$, $S_{22}^{mn} = iS_{22}^{nm}$, $S_{12}^{mn} = iS_{21}^{nm}$ and $S_{21}^{mn} = iS_{12}^{nm}$, where a factor of i has to be

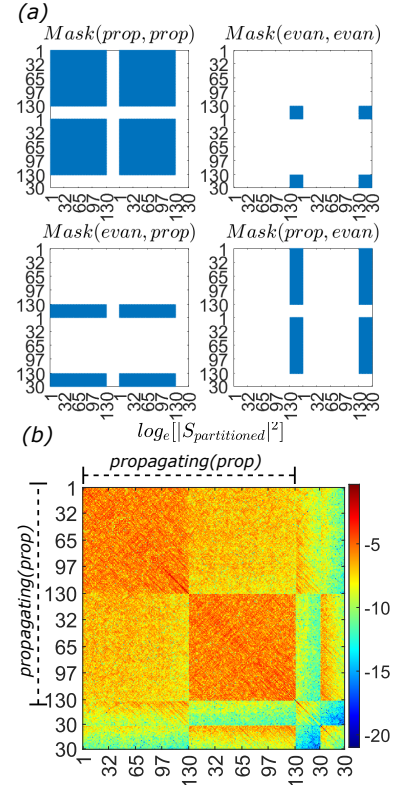


Figure 1.13: The partitioned S matrix. (a) Plotting the sparsity of the selection mask matrix (referred as Mask where the blue colour stands for unity and the white for zeros) used to re-arrange the S matrix given in Figure 1.12 to form a partitioned S matrix ($S_{\text{partitioned}}$) based on [24]. As an example, $\text{mask}(\text{evan}, \text{prop})$ selects that part of the full S matrix which contains only modes such that the incident modes are propagating and the scattered being evanescent. (b) Squared magnitude of the partitioned S matrix [24] in $\log_e$ scale is shown where the matrix elements of the S matrix given in Figure 1.12 is rearranged using the selection mask given in (a) to obtain a form given in equation 1.87. $S_{\text{partitioned}}$ will be used later (as shown in the Figure 1.14) to validate the generalized unitarity and reciprocity relations.

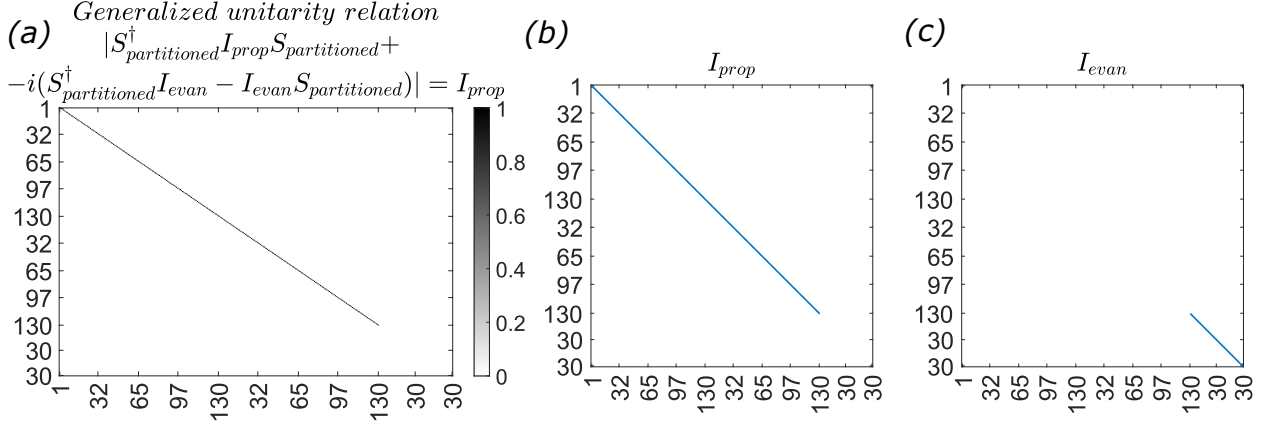


Figure 1.14: Numerical validation of the generalised unitarity relation, involving the S matrix, is demonstrated. (a) Plotting the magnitude of the numerically estimated generalized unitarity relation, based on the analytical result in [24]. All the non-zero diagonal elements (indicative of the propagating modes), are unity, implying the flux conservation. $\dagger$ denotes conjugate transpose. Sparsity of the matrices (b) I_{prop} and (c) I_{evan} , are also shown, where blue colour denotes unity and the white colour for zeros.

incorporated. It also implies that, when $m > M_{prop}$ and $n \leq N_{prop}$, then $S_{11}^{mn} = -iS_{11}^{nm}$, $S_{22}^{mn} = -iS_{22}^{nm}$, $S_{12}^{mn} = -iS_{12}^{nm}$ and $S_{21}^{mn} = -iS_{21}^{nm}$, where a factor of $-i$ has to be incorporated. The numerical validation of the reciprocity relationship, is demonstrated in Figure 1.15.

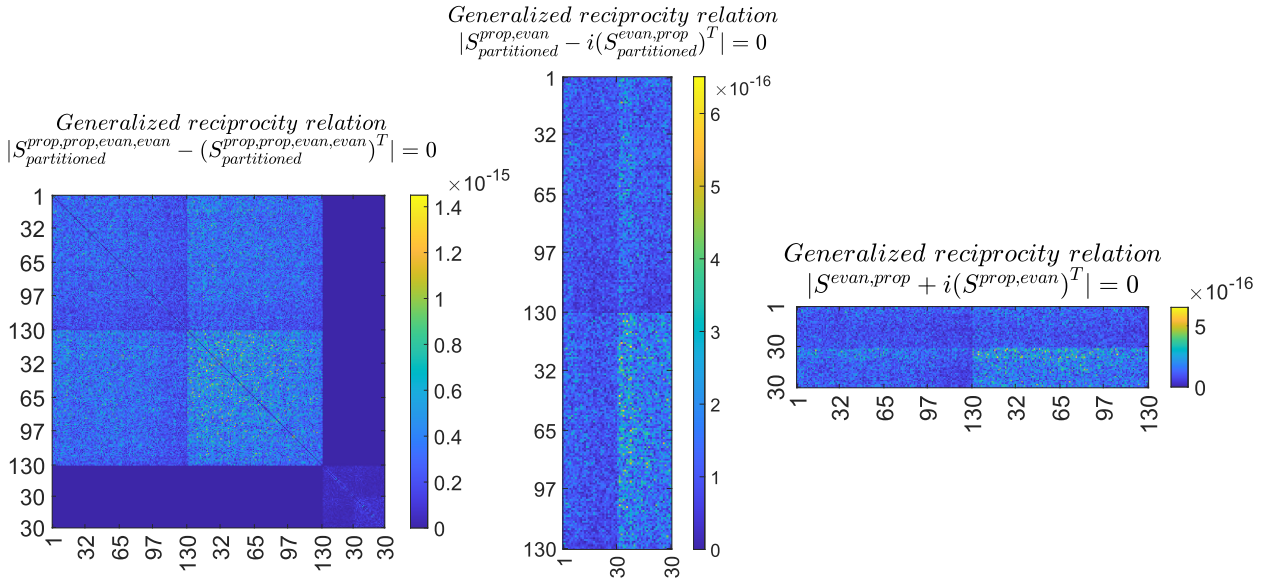


Figure 1.15: Numerical validation of the generalised reciprocity relation, involving the generalised S matrix, is demonstrated. The magnitude of the numerically estimated generalized reciprocity relations, in terms of $S_{partitioned}$, is plotted. T stands for the matrix transpose. $S_{partitioned}^{prop,prop,evan,evan}$ denotes that part of the $S_{partitioned}$ given in equation 1.87, which is a union of $S_{partitioned}^{prop,prop}$ and $S_{partitioned}^{evan,evan}$.

1.5.6 Time-reversal symmetry and the generalised S matrix, containing evanescent modes

For a scattering system obeying the generalised unitarity (obeys energy conservation, without any absorption or gain) and the generalised reciprocity relations, it follows naturally that, such a system would then possess the time reversal symmetry, even for the evanescent wave modes.

For the formal proof, one may refer to [20, 24]. The time reversal phenomenon in the context of monochromatic waves, has to be understood as phase conjugation. At this stage, it is good to define the phase conjugation operation for the propagating and the evanescent modes.

Definition of phase conjugation for the eigenmodes at a boundary plane

For both the propagating and the evanescent wavemodes, let's define a phase conjugation operator, referred to as $PC[.]$, defined with respect to a boundary plane $\Gamma_{L/R}$.

$$\begin{aligned} PC[\psi_m^\pm(z, y)] &= PC[\Phi_m^\pm(z)\chi_m(y)] \\ &= \Phi_m^\mp(z)\chi_m(y) \end{aligned} \quad (1.88)$$

where $\Phi_m^\mp(z)$ is given as

$$\Phi_m^\mp(z) = \begin{cases} \frac{1}{\sqrt{k_z^{(m)}}} e^{\mp i k_z^{(m)} z}, & \text{for the propagating modes} \\ \frac{1}{\sqrt{k_{z, \text{evan}}^{(m)}}} e^{-k_{z, \text{evan}}^{(m)} |z - z_{L/R}|}, & \text{for the evanescent modes at } \Gamma_L \text{ or } \Gamma_R \end{cases} \quad (1.89)$$

One may note that there is no $\mp$ term associated with the evanescent $\Phi_m^\mp(z)$ which is an attenuating real term, for both the cases when $(z - z_{L/R}) > 0$ and $(z - z_{L/R}) < 0$. Therefore, for both the propagating and the evanescent modes,

$$\Phi_m^\mp(z) = (\Phi_m^\pm(z))^* \quad (1.90)$$

where $*$ denotes complex conjugation. Phase conjugation cause the waves to retrace its original path in reverse order converging back at the source, as if time was going backwards.

For a generalised unitary S matrix, time-reversal symmetry relations take the same form as the relations defined for the reciprocity principle, which was numerically validated, as shown in Figure 1.15. As reviewed in the sidenote⁴⁶, such a time reversal symmetry relation, especially involving evanescent wave modes, has paved the way to the sub-wavelength wave focussing applications.

1.6 From the eigenmode basis to the eigenchannel basis : Quasi-1D geometry

As given before in Section 1.5.2, for the wave incidence from the left to the right side of the disorder, the incident wave was represented as $\tilde{E}^{inc} = \sum_m c_m^{inc} \psi_m^+(z, y)$. The corresponding transmitted wave field $\tilde{E}^{trans} = \sum_n t_n^+ \psi_n^+(z, y)$ and the reflected wave field is given as $\tilde{E}^{refl} = \sum_n r_n^- \psi_n^-(z, y)$. The coefficients can be arranged as column vectors

$$\begin{aligned} c^{inc} &= \left(c_1^{inc}, c_2^{inc}, c_m^{inc} \dots c_{M_{total}}^{inc} \right)^T, \quad t^+ = \left(t_1^+, t_2^+, t_n^+ \dots t_{N_{total}}^+ \right)^T, \\ r^- &= \left(r_1^-, r_2^-, r_n^- \dots r_{N_{total}}^- \right)^T, \end{aligned} \quad \text{where } T \text{ denotes matrix transpose. Such a}$$

46: First, let's take the reciprocity relation, involving only the propagating modes. As given towards the end of Section 1.5.5, for the propagating incident and transmitted modes, $S_{21}^{nm} = S_{12}^{mn}$. In words it means, if the m^{th} incident mode is excited at the left side of the disorder and the corresponding complex field transmission of the n^{th} transmitted mode is measured, that complex transmission value will be the same, even if the same n^{th} mode is excited as an incident wave from the right side of the disorder, while measuring the complex transmission associated with the m^{th} transmitted mode on the left. Similarly, the reflectance reciprocity relation $S_{11}^{nm} = S_{11}^{mn}$, can also be put into words. Thus, for a flux conserved scattering system, without any absorption or gain (with a unitary S matrix), the reciprocity relation then naturally implies that, if the reflected and the transmitted modes are excited (as in phase conjugation) sending back into the medium, the originally used incident wave can be regenerated. This is the essence of the time-reversal symmetry relation. Also, there exists [20] reciprocity relations, even between the incident evanescent modes and transmitted propagating modes, as given towards the end of Section 1.5.5. Hence, upon phase conjugation of the propagating waves (in the far-field) transmitted due to an evanescent incident source (near-field), the original evanescent light source can be regenerated, as in a sub-wavelength time-reversed focussing. For the experimental demonstration, one may refer to [22, 43].

[43]: Leroosey et al. (2007), 'Focusing beyond the diffraction limit with far-field time reversal'

[22]: Park et al. (2017), 'Time-reversing a monochromatic subwavelength optical focus by optical phase conjugation of multiply-scattered light'

representation is convenient to describe the wave scattering, in terms of the transmission and reflection matrices, as $t^+ = S_{21}c_{inc}$ and $r^- = S_{11}c_{inc}$. Such a basis expansion⁴⁷ or decomposition of wave scattering, in terms of complex coefficients involving eigenmodes, is referred as the eigenmode basis. As the c_m^{inc} coefficients are generally complex, an arbitrary wave inject unit flux if $\sum_{m=1}^{M_{prop}} |c_m^{inc}|^2 = \|c^{inc,prop}\|^2 = 1$, where $\|\cdot\|$ denotes the Euclidean norm ($\mathcal{L}^2$ norm) of a column vector. The flux normalisation is usually ensured when the incident wave is defined. Although there exist the field transmission and reflection coefficients associated with the purely evanescent incident modes, the corresponding flux transmission and reflection coefficients are left undefined. This is mainly because, the incident evanescent modes alone, as per the mathematical definition, don't inject any flux into the medium. Hence, in this chapter, for flux transmission analysis, particular care is taken not to include the evanescent incident modes. On the other hand, the evanescent incident modes can be used for the estimation of the field transmission and reflection for wavefront shaping applications, without incorporating the flux transmission and reflection analysis.

For a flux normalised incident wave, the flux transmission on the outgoing side, is given as $\tau = \sum_{n=1}^{N_{prop}} |t_n^+|^2 = \|t^{+,prop}\|^2$, as the outgoing eigenmodes are also flux normalised. If one needs to excite all the possible incident propagating eigenmodes at the same time, one may define an incident wave represented by the column vector $c^{inc-all,prop}$, where $c_m^{inc-all,prop} = 1/\sqrt{M_{prop}}$ such that, $\sum_{m=1}^{M_{prop}} |c_m^{inc-all}|^2 = \|c^{inc-all,prop}\|^2 = 1$. Such an incident wave given by $c^{inc-all,prop}$, helps to define the average transmission $\langle\tau\rangle$, where the averaging of the transmission is performed over all the equally-excited propagating modes.

Define average transmission (transmission averaged over all incident propagating eigenmodes excited equally)

For the incident wave (containing only propagating modes) being represented by the column vector $c^{inc-all,prop}$, where the column vector elements $c_m^{inc-all,prop} = 1/\sqrt{M_{prop}}$, $\sum_{m=1}^{M_{prop}} |c_m^{inc-all}|^2 = 1$ and $t^+ = S_{21}c^{inc-all}$, then $\langle\tau\rangle$ ⁴⁸, the average transmission is given as

$$\begin{aligned} \langle\tau\rangle &= \sum_{n=1}^{N_{prop}} |t_n^+|^2 = \frac{1}{M_{prop}} \sum_{m=1}^{M_{prop}} \sum_{n=1}^{N_{prop}} |S_{21}^{nm}|^2 \\ &= \frac{1}{M_{prop}} \text{trace} \{ \{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop} \} \end{aligned} \quad (1.91)$$

A related term, usually encountered in the mesoscopic wave transport theory is the optical conductance g .⁴⁹ For estimating g , all the propagating eigenmodes are equally excited.

Define optical conductance g in the quasi-1D geometry

$$g = \sum_{m=1}^{M_{prop}} \sum_{n=1}^{N_{prop}} |S_{21}^{nm}|^2 = \text{Trace} \{ \{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop} \} \quad (1.92)$$

47: In the optical transmission matrix measurement setup[8] using Spatial Light Modulators (SLM), the basis states (although not a complete basis set) are the Hadamard phase patterns.

48: The given Trace formula, is the main result of [21], also called as the Landauer formalism (refer equation 7.156 of [17]).

49: Refer section 3 of [12] for details. The optical conductance (dimensionless) g , gives an estimate of the total capacity of the system to transport waves as in transmission, through all possible incident eigenmodes being excited with equal weights. Usually $g \gg 1$ in diffusion regime and $g = M_{prop} \langle\tau\rangle$ for the quasi-1D geometry. For the 2D geometry with transverse diffusion, g needs to be evaluated differently as an "expanding waveguide" as given in [44, 45], as the wave transport has additional degrees of freedom to diffuse out, increasing the mentioned capacity, in comparison to the quasi-1D geometry.

1.6.1 Transmission eigenchannels from eigenbasis of $S_{21}^{prop,prop}$

Various aspects of the eigenmode basis were explained in the previous section. The transmission and reflection matrices are transformation mappings for the incident wave expressed in the eigenmode basis to the reflected or the transmitted wave (defined again in the same eigenmode basis). While considering matrix transformations in general, another basis which is frequently used is the “eigenchannel basis”, which is the eigenbasis of the transformation matrix involved. As given in equation 1.91, the transmission properties of the sample are directly associated with the $\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop}$ matrix and not just to the $S_{21}^{prop,prop}$ matrix explicitly (although depending implicitly). A clever way to relate the transmission properties (and thereby to $\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop}$), the transmission matrix (S_{21}) and the eigenchannel basis space, is by the use of the Singular Value Decomposition (S.V.D) [46] of $S_{21}^{prop,prop}$. Although the wave transmission was analysed in the context of the eigenmode basis in all the previous sections, it would be valuable in the following sections, to reformulate the wave transport in the eigenchannel basis. The importance of the eigenchannel basis with respect to wave transport was first put forward by Dorokhov[47], within the context of the coherent electron transport theory, where he proposed that the coherent electron conduction in metals, is mainly due to few highly conducting eigenchannels and most of the remaining eigenchannels are localised (not taking part in the conduction process). This was later explained within the context of the Random Matrix Theory (R.M.T)⁵⁰ by Imry[49], that the wave conductance is mainly due to a small number of effective eigenchannel modes, approximately equal to $g \approx M_{prop} l^* / L$, where M_{prop} is the total number of propagating incident modes as said before, l^* the transport mean free path and L , the longitudinal length of the disordered medium. This concept of the eigenchannels, was later extended to the wavefront shaping of classical waves such as light, for enhancing the total transmission by coupling light into the highly transmitting eigenchannels[2, 6, 50–52]. Next subsection, reviews the the singular value decomposition, eventually leading to the formulation of the eigenchannel basis.

1.6.2 Singular value decomposition and transmission eigenchannels

The singular value decomposition (S.V.D) and the associated eigenchannels are defined with respect to the transmission matrix $S_{21}^{prop,prop}$, which contains only the propagating modes. $S_{21}^{prop,prop}$ of dimension $[N_{prop} \times M_{prop}]$, can be decomposed as

[46]: Mello et al. (1988), ‘Macroscopic approach to multichannel disordered conductors’

[47]: Dorokhov (1984), ‘On the coexistence of localized and extended electronic states in the metallic phase’

[49]: Imry (1986), ‘Active transmission channels and universal conductance fluctuations’

50: For a detailed review of R.M.T within the context of wave scattering in disordered medium, refer to [11] or [48]

[11]: Stone et al. (1991), *Random matrix theory and maximum entropy models for disordered conductors Mesoscopic Phenomena in Solids* ed BL Altschuler, PA Lee and RA Webb

[48]: Garcia-Martin et al. (2005), ‘Statistical properties of wave transport through surface-disordered waveguides’

Singular Value Decomposition (S.V.D)

$$\begin{aligned}
S_{21}^{prop,prop} &= U \Sigma V^\dagger \\
&= \begin{pmatrix} u_{11} & u_{12} & \dots & u_{1N_{prop}} \\ u_{21} & \dots & \dots & u_{2N_{prop}} \\ \dots & \dots & \dots & \dots \\ u_{N_{prop}1} & u_{N_{prop}2} & \dots & u_{N_{prop}N_{prop}} \end{pmatrix} \begin{pmatrix} \sigma_1 & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & 0 \\ 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots \end{pmatrix} \begin{pmatrix} v_{11} & v_{12} & \dots & v_{1M_{prop}} \\ v_{21} & \dots & \dots & v_{2M_{prop}} \\ \dots & \dots & \dots & \dots \\ v_{M_{prop}1} & v_{M_{prop}2} & \dots & v_{M_{prop}M_{prop}} \end{pmatrix}^\dagger \\
&\quad (1.93)
\end{aligned}$$

where U and V are matrices containing the left and the right singular vectors⁵¹ of $S_{21}^{prop,prop}$ and $\sigma_1 = \sqrt{\tau_1}$, $\sigma_2 = \sqrt{\tau_2}$, $\sigma_3 = \sqrt{\tau_3} \dots$ are the singular values such that, $\tau_1 > \tau_2 > \tau_3 \dots$ are the transmission coefficients of the eigenchannels. Therefore, various singular vectors being incident on the sample, creates transmission channels called as eigenchannels with their respectively transmission coefficients. At this stage, it is good to emphasise that a given eigenchannel mode, with a particular transmission (τ_i), is a linear combination of the eigenmodes. The steps taken for visualising the eigenchannels, are given as the following

1.6.3 Visualising the eigenchannels, using the boundary integral equation

Steps for visualising the transmission eigenchannels of S_{21} is given as the following. A similar logic is followed for visualising the eigenchannels of S_{12} .

Steps for visualising the transmission eigenchannels of S_{21}

1. Estimate the generalised transmission matrix S_{21} , using the Fisher-Lee relations (refer table 1.2)
2. Perform S.V.D (refer equation 1.93) on the sub-matrix $S_{21}^{prop,prop}$, which contains only the propagating modes, for both the incident side and the transmitted side.
3. Sort the eigenchannel flux transmission coefficients (τ_i), in the descending order, together with their correspondingly sorted singular vectors. An example for the τ values, for the quasi-1D geometry, is shown in the Figure 1.16.
4. Various columns of the sorted V matrix (or the rows of $V^\dagger$), is used for setting the coefficients for the incident wave, exciting an eigenchannel of the medium, with its corresponding transmission coefficient, τ . As an example, the coefficients of the maximum transmitting eigenchannel on the incident side, is the first singular vector (with the largest transmission coefficient), given as

$$c_{max}^{inc} = \begin{pmatrix} v_{11} \\ v_{21} \\ v_{31} \\ \dots \\ v_{M_{prop}1} \end{pmatrix} \quad (1.94)$$

51: The column vectors contained in U and V are called as the left and the right singular vectors of $S_{21}^{prop,prop}$. The left singular vectors are the orthonormal eigenvectors for $S_{21}^{prop,prop} \{S_{21}^{prop,prop}\}^\dagger$ and the right singular vectors are the orthonormal eigenvectors for $\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop}$. The diagonal Σ matrix contains the same square root of eigenvalues, of both matrices $S_{21}^{prop,prop} \{S_{21}^{prop,prop}\}^\dagger$ and $\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop}$. As $t^+ = S_{21}^{prop,prop} c_{inc}^{inc} = U \Sigma V^\dagger c_{inc}^{inc}$, $V^\dagger$ transforms the incident wavefront in the eigenmode basis space, couples it into the eigenchannel basis space characterised by Σ and U transforms it back into the eigenmode basis space.

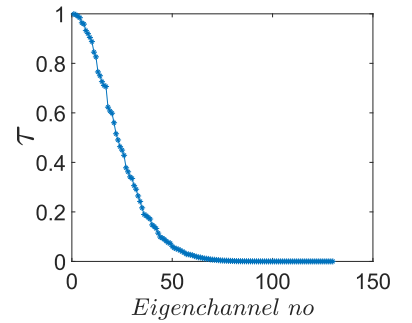


Figure 1.16: Eigenchannel transmission coefficients, are plotted. Eigenchannel transmission coefficients, obtained from the S.V.D of the S_{21} matrix given in Figure 1.12, is plotted. Maximum value of τ is $\tau_{max} = \tau_{i=1} = 0.9991$, the minimum value of τ is $\tau_{min} = \tau_{i=130} = 5.924 \times 10^{-17} \approx 0$ and the average transmission coefficient is $\langle \tau \rangle = 0.1903$.

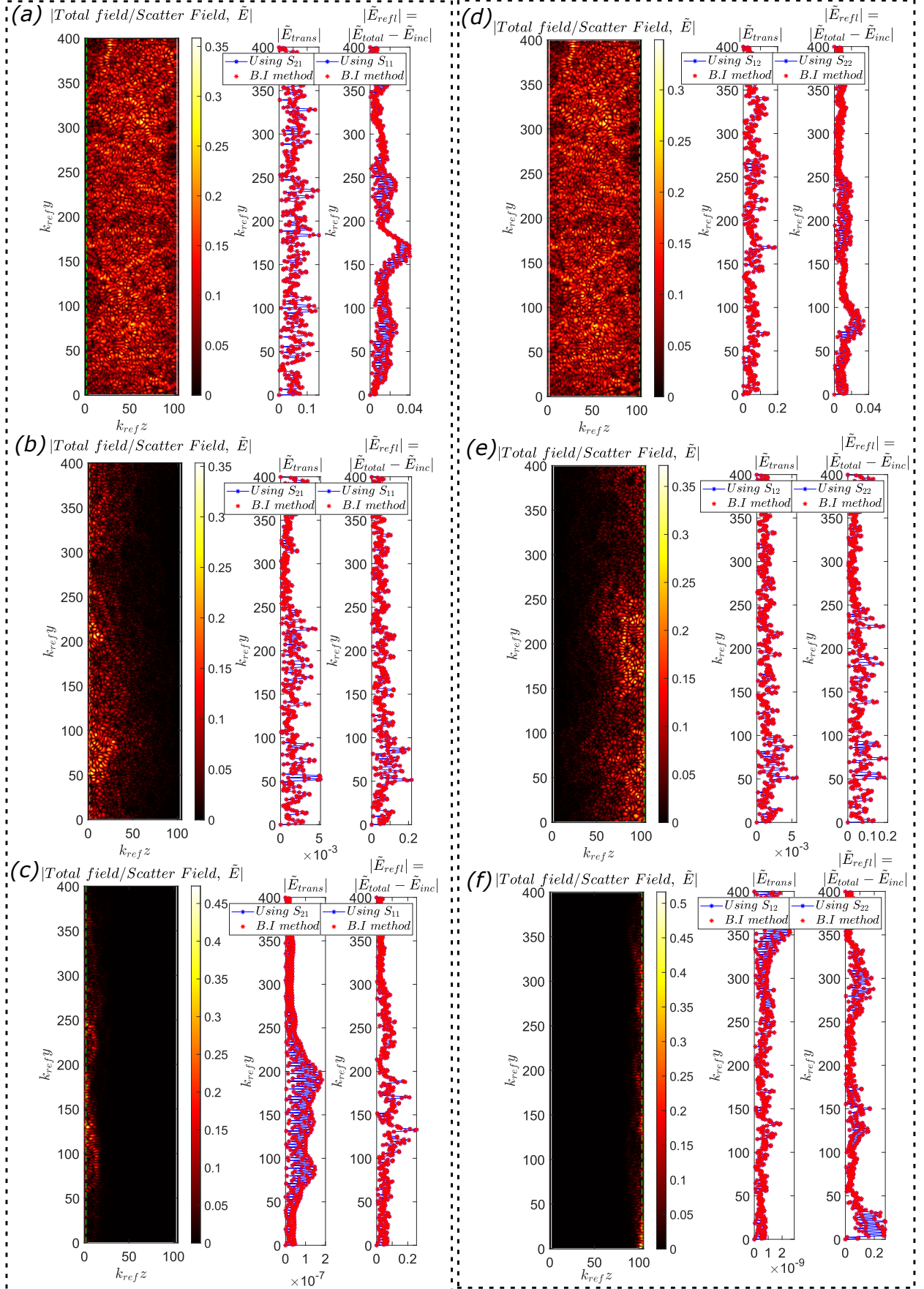


Figure 1.17: Visualising various eigenchannels of S_{21} and S_{12} , containing 130 propagating eigenmodes and 30 evanescent eigenmodes, for the quasi-1D transport problem with $\langle \tau \rangle = 0.1903$. (a) Maximally transmitted (first) eigenchannel of S_{21} , where transmission, $T = 0.9991$ and reflection $R = 0.0009$ (b) An intermediate eigenchannel numbered 86 out of the 130 eigenchannel modes, of S_{21} , where $T = 0.0007$, $R = 0.9993$. (c) Minimally transmitted (last eigenchannel numbered 130) eigenchannel of S_{21} , where $T = 0$, $R = 1$. Similarly, (d) Maximally transmitted (first) eigenchannel of S_{12} , where $T = 0.9991$, $R = 0.0009$ (e) An intermediate eigenchannel numbered 86 out of the 130 eigenchannel modes, of S_{12} , where $T = 0.0007$, $R = 0.9993$. (f) Minimally transmitted (last eigenchannel, numbered 130) eigenchannel of S_{12} , where $T = 0$, $R = 1$. The maximally transmitted eigenchannel of S_{21} and S_{12} looks identical in the inside. It is because the transport path taken from left to right with the maximum transmission close to unity, is the same path taken from right to left for maximal transmission.

such that, due to the orthogonal property of the $V^\dagger$ matrix

$$t_{max}^+ = S_{21}^{prop,prop} c_{max}^{inc} = U \Sigma V^\dagger c_{max}^{inc} = \begin{pmatrix} u_{11} \\ u_{21} \\ u_{31} \\ \dots \\ u_{N_{prop}1} \end{pmatrix} \sigma_1 \quad (1.95)$$

where σ_1 is the largest term in Σ .

5. As the incident modal coefficients are estimated in the previous step, the boundary integral equation (equation 1.81), is used for visualising the eigenchannels, as shown in Figure 1.17. In addition to that, the transmitted and reflected fields estimated with the boundary integral equation, is compared⁵² with respect to the fields estimated from the transmission and the reflection matrices. While comparing, the evanescent part of the generalised transmission and reflection matrices (on the scattered side), are also included, as the boundary integral equation involves the Green's function containing evanescent modes.

Using the above steps, eigenchannels of S_{21} are plotted in Figure 1.17 (a),(b) and (c) and eigenchannels of S_{12} are plotting in Figure 1.17 (d), (e) and (f) respectively, for a given single-realisation of the disorder. As of now, most of the fundamental aspects regarding the formulation of the quasi-1D problem have been discussed. In the following section, the 2D transport problem, incorporating finite sized incident wave modes for accounting transverse diffusion within the slab medium, is discussed. Such a modelling, involving a finite sized beam is important for comparing the results obtained with an experimental scenario, where the beam size would occasionally be smaller than that of the sample thickness L .

1.7 2D transport problem : Accounting transverse diffusion

In order to model the effects of a finite sized incident wave, it is assumed that the incident wave travels through a lead of transverse size D_{in} and then get incident on the disorder, as shown in the Figure 1.18. The incident lead region (region $MNQP$), has the reflecting boundary condition on the transverse boundary (MN and PQ), to contain the wave inside. Once the wave enters the disordered medium (enclosed by the region $ANQOBCA$), it undergoes multiple scattering and transverse diffusion within the slab, relative to the incident wave. The transmission matrix (S_{21}) for the disorder, can be estimated for the quasi-1D geometry (without the lead region $MNQP$) using the Fisher-Lee relation given in table 1.2. This is followed by the estimation of the transmission matrix S_{21}^{lead} of the lead region, without any disorder present anywhere in the whole domain, as given in the following section. Then, the transmission matrix for the 2D transport problem is effectively a matrix multiplication $S_{21}^{2D} = S_{21} S_{21}^{lead}$. S_{21}^{lead} is applicable only for the incident wave modes and not for waves reflected from the region $ANQO$. In other words, the reflected wave doesn't interact with the lead region $MNQP$.

52: In the Figure 1.17, the magnitude of the field distribution is plotted, as per the Total-field/Scatter-field (TF/SF) method[53]. The TF/SF boundary, which is placed on the incident side of the slab, is shown as a dashed green line. The incident field is subtracted from the total field, within the TF/SF region, so that only the scattered field is shown. TF/SF region is the region between the green line and the closest boundary of the computational domain from which, the incident wave emerges.

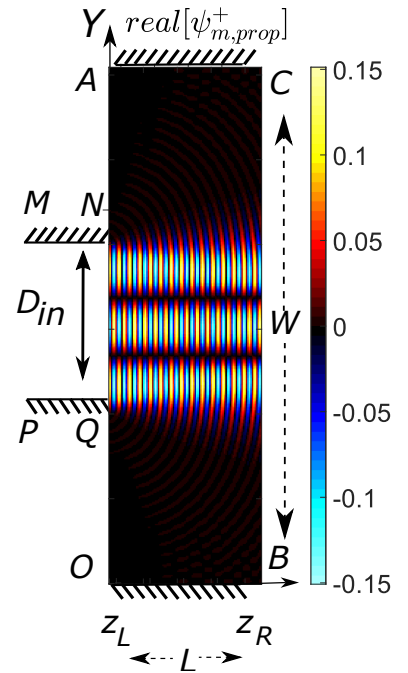


Figure 1.18: Geometry of the 2D transport problem with a finite sized beam incidence is shown. The geometry of the lead region (bounded by reflecting regions MN and PQ) for the incident beam with transverse size D_{in} . Also shown is the m^{th} eigenmode of the lead region ($MNQP$), emerging into the larger domain ($ANQOBCA$) where $m = 3$ and $W/D_{in} = 3$.

1.7.1 Finite sized incident wave modes : A Unitary transformation

There are $M_{prop}^{lead} \approx 2\eta_{ref}D_{in}/\lambda$ propagating eigenmodes within the lead region, where η_{ref} is the reference refractive index taken the same for the lead region Ω_{lead} (enclosed by $MNQP$) and the disorder region Ω (enclosed by $ANQOBC$), to avoid refractive index mismatch between the two regions. There are $M_{prop} \approx 2\eta_{ref}W/\lambda$ modes to be addressed in the disorder region Ω . As usually $D_{in} < W$ in typical experiments, the total transmission matrix $S_{21}^{2D} = S_{21}S_{21}^{lead}$ will be of the dimension $[N_{total} \times M_{prop}^{lead}]$, where N_{total} is the number of transmitted modes in the main region Ω . Next, the methods for estimating S_{21}^{lead} is given. Let the right going, incident propagating eigenmodes in the lead region Ω_{lead} be represented as

$$\psi_{m,prop,lead}^+(z, y)|_{(z,y) \in \Omega_{lead}} = \Phi_{m,prop}^{lead}(z)\chi_m^{lead}(y) \quad (1.96)$$

The field value of the eigenmode at the boundary NQ is given as

$$\psi_{m,prop,lead}^+(z_L, y) = \Phi_{m,prop}^{lead}(z_L)\chi_m^{lead}(y) \quad (1.97)$$

For simplicity, it is assumed in the coding that the segment NQ is centered within the segment AO , such that $AN = QO$ for different values of the lead width D_{in} . Any incident eigenmode has to be continuous at the boundary NQ , which is overlapping with the boundary $ANQO$. Let the eigenmodes in the main disorder region Ω at the boundary $ANQO$ be given as

$$\psi_{n,prop}^+(z_L, y) = \Phi_{n,prop}^{\Omega}(z_L)\chi_n^{\Omega}(y) \quad (1.98)$$

Let the m^{th} eigenmode in the lead boundary NQ be expressed as a summation of eigenmodes in the disorder region (Ω)

$$\Phi_{m,prop}^{lead}(z_L)\chi_m^{lead}(y) = \sum_{j=1}^{M_{prop}} d_j \Phi_j^{\Omega}(z_L)\chi_j^{\Omega}(y) \quad (1.99)$$

Therefore, for a given eigenmode in the lead, d_j can be estimated using the orthogonality relationship involving $\chi_j^{\Omega}(y)$. Integrating the both sides of equation using $\chi_{j'}^{\Omega}(y)$ to invoke orthogonality,

$$\begin{aligned} \langle \chi_{j'}^{\Omega}(y) | \Phi_{m,prop}^{lead}(z_L)\chi_m^{lead}(y) \rangle &= \\ \langle \chi_{j'}^{\Omega}(y) | \sum_{j=1}^{M_1} d_j \Phi_j^{\Omega}(z_L)\chi_j^{\Omega}(y) \rangle &= d_{j'} \Phi_{j'}^{\Omega}(z_L) \end{aligned} \quad (1.100)$$

Therefore, the coefficient $d_{j'}$ can be estimated as

$$d_{j'} = \frac{1}{\Phi_{j'}^{\Omega}(z_L)} \langle \chi_{j'}^{\Omega}(y) | \Phi_{m,prop}^{lead}(z_L)\chi_m^{lead}(y) \rangle \quad (1.101)$$

For a given m value, a column of coefficients $d_{j'}$ can be estimated. For different m values, a matrix can be formed which is the $S_{21}^{lead}(j', m)$ matrix. $S_{21}^{lead}(j', m)$ is a unitary matrix, which preserves the norm of the incident wave coefficients (a column vector), with respect to the transmitted wave coefficients of S_{21}^{lead} . Hence, $S_{21}^{lead}(j', m)$ prevents any loss during this

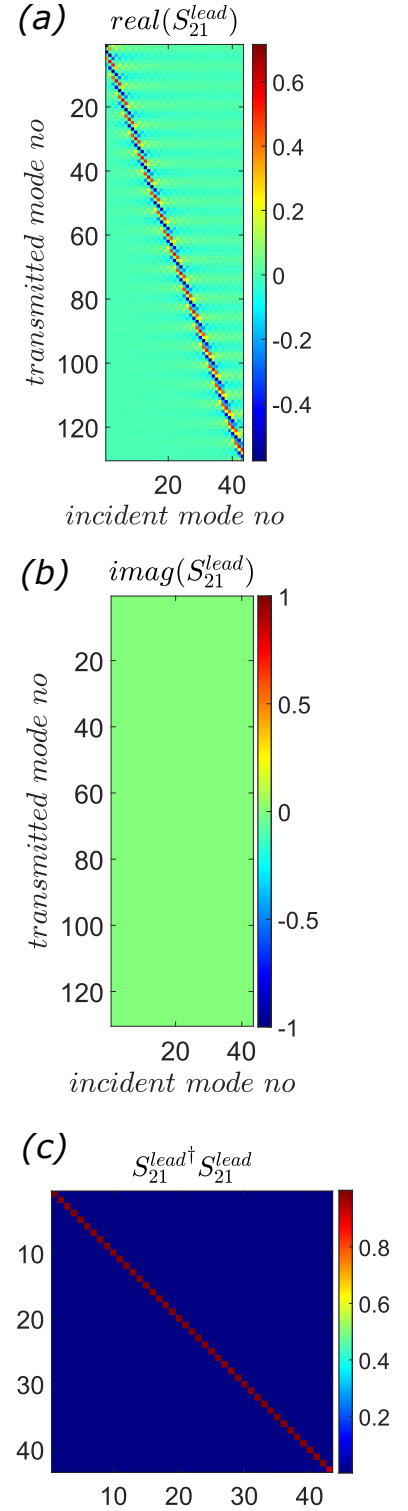


Figure 1.19: Plotting S_{21}^{lead} for the 2D transport problem. $W/D_{in} = 3$, $M_{prop}^{lead} = 43$ and $M_{prop} = 130$. (a) Real part of S_{21}^{lead} (b) Imaginary part of S_{21}^{lead} and (c) Showing the unitarity property of the S_{21}^{lead} lead that $S_{21}^{lead\dagger} S_{21}^{lead} = I$, implying there is no loss in the diffraction process from the lead region $MNQP$ to the region $ANQOBCA$.

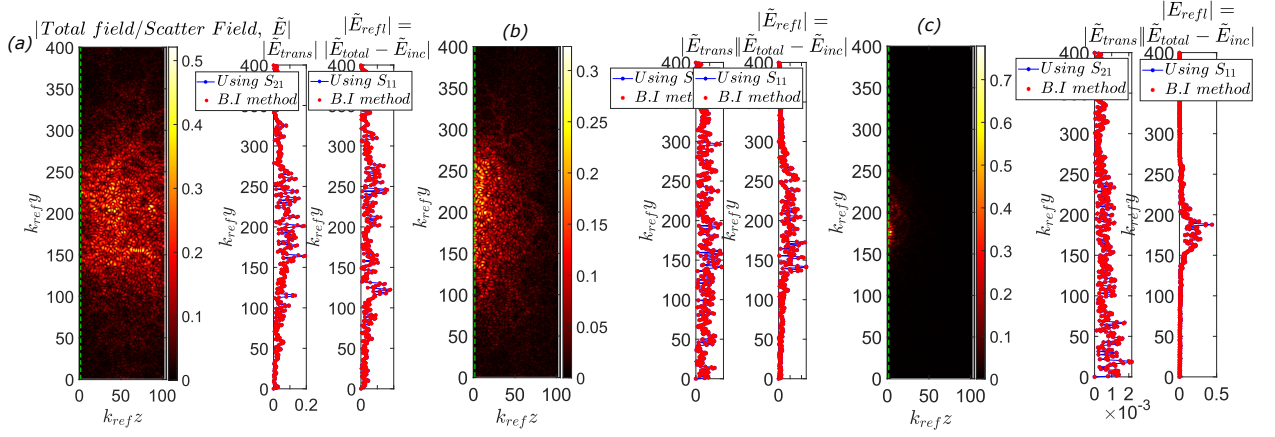


Figure 1.20: Eigenchannels for a finite sized beam, as in a 2D transport problem, obtained from the S.V.D of the $S_{21}^{2D} = S_{21}S_{21}^{lead}$ matrix, are plotted, where $\langle \tau \rangle = 0.1827$. (a) Maximum transmitting eigenchannel (first eigenchannel) for a finite sized beam is plotted. Magnitude of the total-field/scatter-field, due to the maximally transmitted eigenchannel is shown, where total transmission, $T = 0.8243$ and $R = 0.1746$. (b) An intermediate eigenchannel (numbered 28) is shown, where $T = 0.0149$ and $R = 0.9822$ (c) Minimally transmitted eigenchannel (eigenchannel number 43) is plotted, where $T = 0.0001$ and $R = 0.9998$. S_{21}^{lead} used, is shown in Figure 1.19, where $W/D_{in} = 3$. For the eigenchannel transmission coefficients, refer to Figure 1.21.

transformation, when the incident waves transforms through the lead, diffracting into the disorder region. An example for $S_{21}^{lead}(j', m)$ estimated, is plotted in Figure 1.19.

1.7.2 Eigenchannel basis for the 2D transport problem

Once the effective transmission matrix ($S_{21}^{2D} = S_{21}S_{21}^{lead}$), incorporating the finite size of the incident modes is obtained, then the S.V.D can be performed on the matrix to obtain the eigenchannel basis for the 2D transport problem. The field profile associated eigenchannels (the maximally transmitted, an intermediately transmitted and the minimally transmitted) for a given single-realisation of the disorder, are shown in Figure 1.20 (a), (b) and (c), respectively. As given in the Figure 1.21, the maximally transmitted eigenchannel and minimally transmitted eigenchannel, don't have the quasi-1D transmission values of 1 and 0, respectively. This is due to the reduction in "controllability" as described in [2, 3, 15], caused due to the transverse diffusion (spreading of waves relative to the beam size and longitudinal thickness, L of the slab) of waves, occurring inside the slab, in comparison to the quasi-1D wave transport. Such of notion of wavefront shaping controllability[2, 3, 15] is conceptually intertwined with the idea of long-range wave correlations[14] through the diffusive medium.

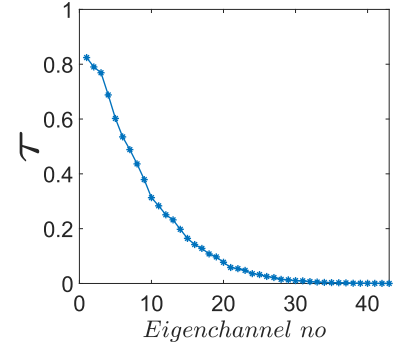


Figure 1.21: Eigenchannel transmission coefficients, for the 2D transport problem, obtained from the S.V.D of the $S_{21}^{2D} = S_{21}S_{21}^{lead}$ matrix, are plotted. Maximum value of τ is $\tau_{max} = \tau_{i=1} = 0.8243$, the minimum value of τ is $\tau_{min} = \tau_{i=43} = 0.0001$ and the average transmission coefficient is $\langle \tau \rangle = 0.1827$. S_{21}^{lead} is shown in Figure 1.19, where $W/D_{in} = 3$. It can be inferred that, the maximally transmitted eigenchannel and minimally transmitted eigenchannel, don't have the quasi-1D transmission values of 1 and 0, respectively.

1.8 Cascading of the generalised scattering matrices

This section explains the S matrix cascading method by which, a larger disordered slab can be formed, by cascading an ensemble of thinner slabs. Cascading of the generalised S matrices of the thinner slabs, builds the sample along the longitudinal dimension (z axis) step-by-step, as shown in the schematic given in Figure 1.22. It can be seen from Figure 1.22(b)

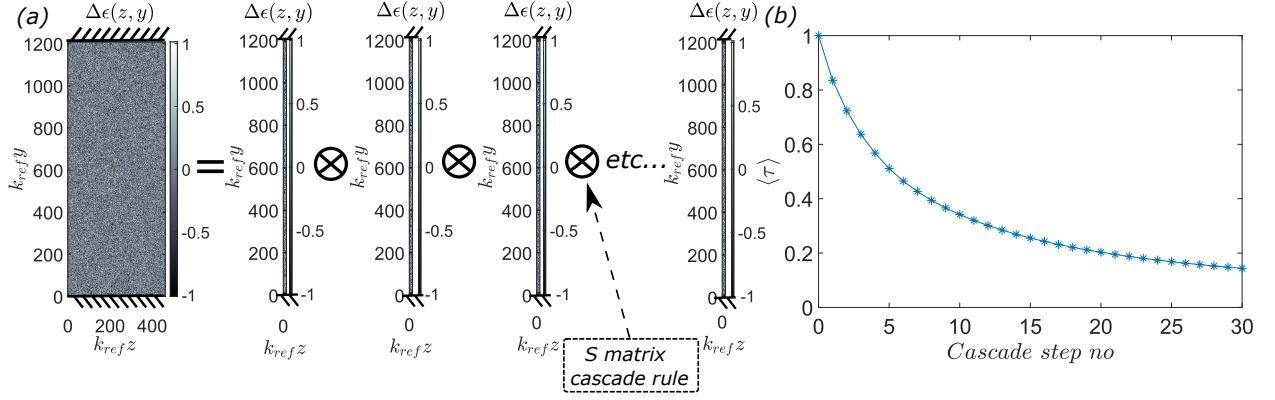


Figure 1.22: Schematic to demonstrate the S matrix cascade rule is shown. (a) Schematic of cascading thinner slabs to form thicker slab is shown. Cascade rule given in equation 1.104 is used to cascade the slabs. First, the first and the second thin slabs are cascaded. It is followed by cascading the third slab with the cascaded result obtained from the first and the second slab. This pattern is repeated, until the last thin slab is cascaded. **(b)** The ensemble averaged total transmission $\langle \tau \rangle$ of the cascaded slabs as a function of the step number of cascading (30 thin slabs are cascaded) is plotted. The ensemble averaged transmission profile is obtained by the random shuffling of the order of the thin slabs taken for cascading.

that, the transmission profile as a function of cascading step size (or the longitudinal sample size L), follows a diffusion law whose analytic form is given in chapter 3. Different realisations of thicker slabs (200 in number) can be formed from the same S matrices of the thinner slabs (30 in number), taken in random order.⁵³ Cascading method⁵⁴ for S matrices is given as the following

$$S^{(a)} = \begin{pmatrix} S_{11}^{(a)} & S_{12}^{(a)} \\ S_{21}^{(a)} & S_{22}^{(a)} \end{pmatrix} \quad (1.102)$$

and

$$S^{(b)} = \begin{pmatrix} S_{11}^{(b)} & S_{12}^{(b)} \\ S_{21}^{(b)} & S_{22}^{(b)} \end{pmatrix} \quad (1.103)$$

$$S^{\text{cascade}} = S^{(a)} \otimes S^{(b)} = \begin{pmatrix} S_{11}^{(a)} & S_{12}^{(a)} \\ S_{21}^{(a)} & S_{22}^{(a)} \end{pmatrix} \otimes \begin{pmatrix} S_{11}^{(b)} & S_{12}^{(b)} \\ S_{21}^{(b)} & S_{22}^{(b)} \end{pmatrix} \\ = \begin{pmatrix} S_{11}^{(a)} + S_{12}^{(a)} (I - S_{11}^{(b)} S_{22}^{(a)})^{-1} S_{11}^{(b)} S_{21}^{(a)} & S_{12}^{(a)} (I - S_{11}^{(b)} S_{22}^{(a)})^{-1} S_{12}^{(b)} \\ S_{21}^{(b)} (I - S_{22}^{(a)} S_{11}^{(b)})^{-1} S_{21}^{(a)} & S_{22}^{(b)} + S_{21}^{(b)} (I - S_{22}^{(a)} S_{11}^{(b)})^{-1} S_{22}^{(a)} S_{12}^{(b)} \end{pmatrix} \quad (1.104)$$

where I is the identity matrix⁵⁵. The S matrices for a collection of the smaller slabs, are estimated serially using the Fisher-Lee relations, as explained before, followed by the use of the cascading formula given in equation 1.104. Upon obtaining a comparatively larger sample along the transverse dimension (y axis), the S matrix obtained would also be larger, with respect to the number of propagating modes. This helps to analyse the nature of the transmission matrix from a statistical point of view, which would be discussed in the following section.

53: This is particularly advantageous from a computational point of view that, one need not model 200 different large slabs, but could estimate the S matrices of a collection of smaller slabs once and cascade them using random order of the slabs, for obtaining different realisations of larger slabs.

54: Refer 2.5.1.1 of [54] for the derivation.

[54]: Jin (2014), 'New Methods and Theory for Increasing Transmission of Light through Highly-Scattering Random Media.'

55: The cascading formula is particularly stable, because of the identity matrix appearing inside the matrix inversion terms contained within equation 1.104.

1.9 Statistical aspects for testing and validation of the developed code

This section reviews the ensemble averaged statistical properties associated with the propagating $S_{21}^{prop,prop}$ of the larger cascaded slabs for the quasi-1D transport problem, involving many realisations of the disorder. The main goal of this section would be to use the statistical aspects of the random $S_{21}^{prop,prop}$ matrix, for testing and validating the code developed for modelling. Although the quasi-1D transport problem is a very important field of study, its experiment relevance in wave physics is mostly restricted to microwave experimental geometries[16]. However, in this chapter the importance of quasi-1D transport statistics is that, the statistical aspects of the eigenchannel transmission distribution is analytically known and could provide a method for testing and validating the statistical aspects associated with modelled of $S_{21}^{prop,prop}$.

1.9.1 Quasi-1D transport problem and random matrix theory : Moments and cumulants

For the quasi-1D transport geometry, the eigenchannel transmission distribution takes the form of a bimodal distribution, which is analytically known⁵⁶ and can be estimated using the modelled $S_{21}^{prop,prop}$, as shown in the Figure 1.23. One way to characterise a probability density function (such as the eigenchannel transmission distribution) is by its moments⁵⁷ or cumulants.⁵⁸ As the probability density function of eigenchannel transmission distribution is analytically known for the quasi-1D transport problem, the moments and cumulants of the eigenchannel transmission distribution can also be estimated. As the values can be estimated analytically, it could be used to validate the moments and cumulants estimated from the modelled framework. Mathematica[®] is used to estimate moments and cumulants of the analytical transmission probability distribution, given in equation 1.105. The ensemble averaged value of $\langle \tau \rangle$, estimated from the modelling, is substituted in the analytically estimated expressions for the moments and the cumulants. This is compared against the numerically estimated moments (using the histogram of data) and cumulants (using the expectation operators on the data), to validate the results. The ensemble averaged moments and cumulants of the bimodal distribution (Quasi-1D transport problem using cascaded S matrix), are given in the tables 1.5 and 1.6, respectively. 200 samples are used for ensemble averaging the moments and cumulants, using the eigenchannel transmission values.

Table 1.5: Moments of the bimodal distribution

Moments	Expression	Analytical	Modelling
m_1	$\langle \tau \rangle$	0.1441	0.1456
m_2	$\frac{2}{3} \langle \tau \rangle$	0.0961	0.0954
m_3	$\frac{8}{15} \langle \tau \rangle$	0.0769	0.0758
m_4	$\frac{16}{35} \langle \tau \rangle$	0.0659	0.0647

56: Quasi-1D eigenchannel probability density function from the Random Matrix Theory (R.M.T)[18, 55]

$$p(\tau) = \frac{1}{2} \frac{L^*}{L} \frac{1}{\tau \sqrt{1-\tau}} \approx \frac{1}{2} \langle \tau \rangle \frac{1}{\tau \sqrt{1-\tau}} \quad (1.105)$$

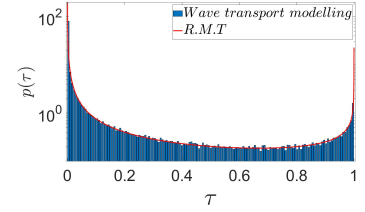


Figure 1.23: Bimodal eigenchannel transmission distribution for the quasi-1D transport: Modelled data vs the analytical distribution, given in equation 1.105, is plotted. Here, $\langle \tau \rangle = 0.144145$ and the disorder taken, is shown in Figure 1.22. Average histogram of 200 samples are taken for estimating the ensemble averaged probability density function. The histogram (no of bins taken is 150) obtained from the modelling is normalised such that $\int p(\tau) d\tau = 1$. The comparison of moments and cumulants, between the modelled distribution and the analytical distribution, are given in tables 1.5 and 1.6, respectively. There are 392 propagating modes involved and the average dimensionless correlation length of $k_{ref} l_c = 0.8613$. The aspects of spatial correlation will be covered in Chapter 2.

57: Moments of a probability density function $p(\tau)$

$$\begin{aligned} m_1 &= \int \tau p(\tau) d\tau \\ m_2 &= \int \tau^2 p(\tau) d\tau \\ m_3 &= \int \tau^3 p(\tau) d\tau \\ m_4 &= \int \tau^4 p(\tau) d\tau \text{ etc...} \end{aligned} \quad (1.106)$$

58: Cumulants of $p(\tau)$ in terms of moments

$$\begin{aligned} k_1 &= \text{mean} = E(\tau) = m_1 \\ k_2 &= \text{variance} = E \left\{ (\tau - E(\tau))^2 \right\} = m_2 - m_1^2 \\ k_3 &= \text{skewness} = E \left\{ (\tau - E(\tau))^3 \right\} \\ &= m_3 - 3m_1 m_2 + 2m_1^3 \\ k_4 &= \text{kurtosis} = E \left\{ (\tau - E(\tau))^4 \right\} - 3k_2^2 \\ &= m_4 - 3m_2^2 - 4m_1 m_3 + 12m_1^2 m_2 - 6m_1^4 \end{aligned} \quad (1.107)$$

where $E()$ denotes the expectation.

Table 1.6: Cumulants of the bimodal distribution

Cumulants	Expression	Analytical	Modelling
mean	$\langle \tau \rangle$	0.1441	0.1441
variance	$-\langle \tau \rangle^2 + \frac{2}{3} \langle \tau \rangle$	0.0753	0.0748
skewness	$2\langle \tau \rangle^3 - 2\langle \tau \rangle^2 + \frac{8}{15} \langle \tau \rangle$	0.0413	0.0407
kurtosis	$-6\langle \tau \rangle^4 + 8\langle \tau \rangle^3 - \frac{52}{15} \langle \tau \rangle^2 + \frac{16}{35} \langle \tau \rangle$	0.0152	0.0149

The modelled results⁵⁹ and the analytical results are within reasonable agreement.

1.10 Conclusion

The main contribution of this chapter is the development of the analytical and the computational code framework, for the estimation of the generalised S matrix, using the extended (generalised) Fisher-Lee relations, suitable for wavefront shaping applications. The generalised S matrix enables to completely characterise the scattering response of a disorder, inclusive of the evanescent modes which are important for the near-field imaging applications. Correctness of the codes developed for generating the S matrices, is validated by **1)** testing out the analytically known generalised unitarity and reciprocity relationships, against the numerically estimated S matrix, **2)** using the Kirchhoff-Helmholtz boundary integral formulation for visualising the reflected and the transmitted waves, which are matched to the scattered waves estimated by the S matrix and **3)** validating the eigenchannel probability density function estimated using the code, against the analytically known results. Cascading of the generalised S matrices presented in the chapter is advantageous as it **1)** helps to parallelise the problem by estimating the S matrix of a larger sample, by breaking it into thinner slabs and estimating their S matrices for cascading, **2)** helps to easily perform ensemble averaging, by randomly shuffling the order of the S matrices of the thinner slabs during the cascading process, **3)** helps to overcome the larger memory requirement for storing the Green's function, otherwise required for a larger slab and **4)** enables the cascading of slabs by incorporating the evanescent modes. Although, the numerical modelling and the analytical methods were described for the $2D$ scalar wave transport problem, the methods can be generalised to the $3D$ scalar or vector wave transport problem, as the Green's function, the boundary integral formulations and the basis wave modes are very general concepts in physics. Finally, it is worth to point out that statistical properties of the S matrices such as the eigenchannel distribution or the generalised unitarity and reciprocity relations, are the same for both $2D$ and $3D$ transport problems, in the diffusion regime.

59: For the moments given in table 1.5, $\langle \tau \rangle$ is estimated by averaging the eigenchannel transmission coefficient, estimated from 200 transmission matrices. For the modelled data, the probability density function of the eigenchannel distribution as a histogram is estimated, followed by estimation of the moments from the obtained histogram. For the cumulants given in table 1.6, $\langle \tau \rangle$ is estimated the same as before. The modelled cumulants are estimated by using the expectation operators as given before, acting on the estimated eigenchannel transmission coefficient distribution.

Comparison between wave transport and diffusion theories

2

2.1 Introduction

A comparative study exploring the inter-relationships between different light transport modelling formalisms in random media is presented in this chapter. Conventionally, two kinds of modelling approaches are employed for estimating light transport profiles in random media. The first kind of approach uses the phenomenological radiative transport equation (*R.T.E*)[56] for macroscopic media, which addresses the aspects of the energy diffusion. The *R.T.E* can be simplified by its diffusion approximation¹ or can be generally solved using the Monte-Carlo technique², which again addresses the classically incoherent transport aspects. On the other hand, the statistically coherent³ transport aspects in random media such as coherent (mean-field) transmission, speckle correlations[14], weak localisation and coherent backscattering[62] are absent within the conventional diffusion theory. For studying such coherent aspects, which is relevant in the context of wavefront shaping, a second approach commonly referred to as the mesoscopic[17] wave transport theory and modelling is needed.

The main goal and contribution of this chapter is to compare the coherent (mesoscopic) wave transport model involving the *S* matrix cascading (given in Chapter 1) and the spatially correlated disorders (to be explained in this chapter), with that of the classically incoherent transport theory involving the diffusion theory. The Quasi-1D problem of estimating the transport properties from an ensemble of transmission matrices for spatially uncorrelated disorders, has been reported by Zhi and Genack[63]. It helps in understanding the relationship between the transmission matrices and the diffusion theory, especially in the semi-ballistic (translucent) regime. The associated transmission scaling law in terms of (L/l^*) (where L is the longitudinal thickness and l^* , the transport mean-free path) of the slab medium, helps to predict the wave transport behaviour of large (centimeter sized) samples for which it is prohibitively harder to model the wave scattering behaviour. In the first part of the chapter, it is attempted to model the link between ensemble averaged parameters involving wave fields, scattering mean free path (l) and spatially correlated disorders, with the disorder correlation length l_c . As diffusion models deal with ensemble averaged parameters which are not specific to a particular realisation of the disorder (e. g. l and l^*), ensemble averaging needs to be used in wave transport modelling to compare it with diffusion model. In the following section, the ensemble averaged wave field (also called as the statistically coherent component of the wave field)⁴ is reviewed to connect it with scattering mean free path (l), disorder correlation length (l_c) and *S* matrix cascading in non-absorbing media. After that, the effect of l_c on the classically “incoherent” (diffusive) intensity and l^* , for spatially correlated disorders is discussed.

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1: For learning the diffusion model for wave transport in detail, refer chapter 5 of [57], chapter 9 of [58], chapter 4 and 5 of [59] and most importantly, chapter 5 of [17].

2: For the Monte Carlo methods, chapter 3 of [57], [60] and [61].

3: The term “statistical coherence” associated with ensemble averaging, should not be confused with the notion of the classical coherence of wave sources. Classical coherence of wave sources, gives the waves their ability to interfere and form interference/speckle patterns. In this thesis, the modelling always use such coherent wave sources. On the other hand, the word “coherence” used in the context of ensemble averaging of random media, denotes those physical entities which don’t average to zero over disorder ensemble averaging. Few examples are, the coherent (mean-field) intensity inside an effective medium, the short and long range correlations, coherent back-scattering etc... which don’t get averaged to zero, upon ensemble averaging. In other words, these “coherent” aspects, survive ensemble averaging, to have a finite non-zero value.

4: For learning more about the ensemble averaged mean-field(also called as statistically coherent component of the wave field), refer to the original paper by Foldy [64], the follow up paper by Lax[65], section IV, V and VI of [30], chapter 4 of [66], chapter 5 (section 3) of [67] and [68].

2.2 Statistically coherent wave field (ensemble averaged mean-field) and the incoherent (diffusive) intensity

Before getting into the mathematical form of the coherent mean field and its associated spatial extinction in the effective medium to obtain l , a pedagogical introduction to the coherent mean-field is given. The Figure 2.1 shows the effect of the progressive increase of turbidity on the light propagation through a random medium. Upon adding lipid like substance in steps to clear water, the incident laser beam transmission through the petri dish undergoes a crossover from the purely ballistic to highly diffusive transport regimes. A transmission crossover regime is

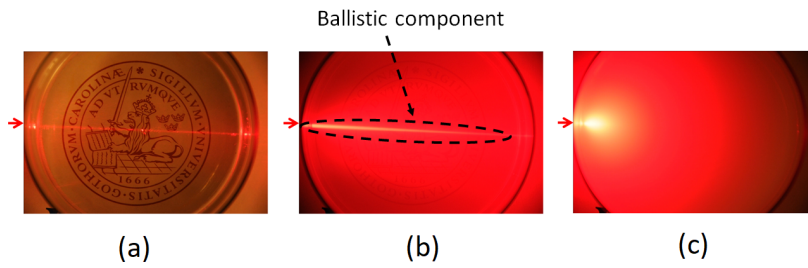


Figure 2.1: Different regimes of light diffusion in random media. (a) The purely ballistic regime where the incident laser beam propagates in clear water. (b) On adding lipid like substance to the clear water, the light beam starts to cross over from the ballistic regime to the diffusion regime. (c) The diffusion regime, where high turbidity forces light to undergo diffusion. The image courtesy is attributed to Prof. Stefan Andersson-Engels.

shown in Figure 2.1 (b), where both the ballistic and the diffusive part of the incident beam are visible. The ballistic component is shown within the dashed curve, outside of which is the diffused component of the incident beam due to random scattering. In Figure 2.1(c), due to the high turbidity, the ballistic component undergoes spatial extinction at a short distance from the incident surface of the medium. Figure 2.1 (b) shows the intensity of the scattered wave. To imagine the associated wave field for a given disorder, fluctuating field values around the mean value of zero need to be considered. Then, on ensemble averaging of the field values for many disorder realisations, the coherent mean-field inside the disorder is obtained. The coherent mean-field has a similar visual resemblance⁵ to the ballistic component shown within the dashed curve, as it is the ballistic part of the incident beam which sustains the ensemble averaging without getting averaged to zero. However, upon ensemble averaging for estimating the coherent component, this diffusive field component formed due to the scattering of the incident beam, gets averaged to zero due to the random field fluctuations around the zero value. Hence, the scattering mean free path l of a non-absorbing medium is defined as the extinction length (in an effective medium) in which, the intensity of the coherent mean-field gets attenuated by $1/e$ [69]. Applying ensemble averaging on the equation 1.81 given in Chapter 1, the expression for the coherent mean-field can be obtained as the following

5: Although the coherent mean-field has resemblance to that of the ballistic field shown in Figure 2.1(b) for a given disorder realisation, they are quantitatively different from each other due to the involvement of ensemble averaging for estimating the mean-field.

[69]: Ishimaru et al. (1982), 'Attenuation constant of a coherent field in a dense distribution of particles'

Coherent intensity and the scattering mean-free path

Coherent (mean-field) component is given as,

$$\langle \tilde{E}(z_0, y_0) \rangle|_{(z_0, y_0) \in \Omega} = \sum_{m=1}^{M_{total}} 2ik_z^{(m)} \int \tilde{E}_m^{inc}(z, y) \langle G(z, y, z_0, y_0) \rangle|_{(z, y) \in \Gamma_L} dy \quad (2.1)$$

where $\tilde{E}_m^{inc}(z, y)|_{(z, y) \in \Gamma_L} = c_m^+ \psi_m^+(z, y)|_{(z, y) \in \Gamma_L}$ is a deterministic term and $\langle \dots \rangle$ denotes ensemble averaging. The coherent intensity is given as

$$I_{coh}(r) = |\langle \tilde{E}(r) \rangle|^2 \quad (2.2)$$

Usually, the y integrated coherent intensity undergoes the Beer-Lambertian transmission within an effective slab medium with an extinction length of l , where l is the scattering mean-free path.

$$I_{coh}(z) = I_0 e^{-z/l} \quad (2.3)$$

where $I_0 = I(z = 0)$ is the peak intensity.

Although the scattering mean-free path l is defined with respect to the coherent intensity in the above equation, in this chapter l won't be estimated by fitting the intensity attenuation within the medium. This is because, ensemble averaging (involving 100s of samples) to estimate the coherent intensity attenuation inside the slab medium is computationally expensive. Instead, the cascading of S matrices by random shuffling the cascading order to generate ensembles of S matrices will be used in this chapter. To be precise, the evolution of the coherent component of the total transmission upon the S matrix cascading will be used to estimate l . Nevertheless, equation 2.1 could be used for visualising the coherent mean field inside the effective medium.

Until now, the scattering mean free path (l) was phenomenologically defined, but the actual physical phenomenon which parametrises l is reviewed in the following sections of the chapter. The physical origin of l is associated with the spatial correlation length (l_c) and the associated disorder randomness power spectrum, which causes the coherent mean-field to attenuate within the disorder. On the other hand, the total transmission profile of the incoherent or the diffused component doesn't obey a simple Beer-Lambert law (like that of 2.3) but obeys the standard diffusion equation [10, 70] involving another transport parameter called as the transport mean free path l^* , which will be discussed in second half of the chapter. To connect the incoherent (diffuse) intensity with that of the total wave field $\tilde{E}(z_0, y_0)$, what has been done historically⁶ is to first define the following two-point field correlation function and then take the limit where the two points converge together to a single point in space, together with the condition that $z/l^* > 3$ [71] (for the quasi-1D geometry) to be in the diffusion regime.

[70]: Durian (1994), 'Influence of boundary reflection and refraction on diffusive photon transport'

[10]: Rossum et al. (1999), 'Multiple scattering of classical waves: microscopy, mesoscopy, and diffusion'

6: The use of the field correlation functions and its connection to radiative transport in random media, was popularised by the perturbation theory of Frish[30] and Tatarskii et al.[66]. The Green's function field correlation contained in the field correlation function for random media, given in equation 2.4, satisfies the Bethe-Salpeter equation. Derivation of the diffusion approximation from the Bethe-Salpeter equation involving field correlation, is provided in Carminati and Schotland[19] Section 24.3.

[71]: Zhang et al. (1999), 'Wave transport in random media: The ballistic to diffusive transition'

Incoherent(diffuse) intensity and the transport mean-free path

Field correlation function is given as

$$\langle \tilde{E}(z_0^{(1)}, y_0^{(1)}) \tilde{E}^*(z_0^{(2)}, y_0^{(2)}) \rangle |_{(z_0^{(1)}, y_0^{(1)}, z_0^{(2)}, y_0^{(2)}) \in \Omega} = \int \int \langle G(z, y^{(1)}, z_0^{(1)}, y_0^{(1)}) G^*(z, y^{(2)}, z_0^{(2)}, y_0^{(2)}) \rangle E_{inc}(z, y^{(1)}) E_{inc}^*(z, y^{(2)}) dy^{(1)} dy^{(2)} |_{(z, y^{(1)}, y^{(2)}) \in \Gamma_L} \quad (2.4)$$

where $E_{inc}(z, y) = \sum_{m=1}^{M_{total}} 2ik_z^{(m)} \tilde{E}_m^{inc}(z, y)$ is the incident wave which is a deterministic term. Then, the incoherent (diffuse) intensity $P_d(r)$ is defined⁷ as the following limit of the field correlation function,

$$P_d(r) = \lim_{(r_0^{(1)} \rightarrow r_0^{(2)})=r} \langle \tilde{E}(r^{(1)}) \tilde{E}^*(r^{(2)}) \rangle |_{(r^{(1)}, r^{(2)}) \in \Omega} = \langle \tilde{E}(r) \tilde{E}^*(r) \rangle |_{(r) \in \Omega} = \langle |\tilde{E}(r)|^2 \rangle |_{(r) \in \Omega} \quad (2.5)$$

where r is in the diffusion regime and $P_d(r)$ obeys the following diffusion equation in a non-absorbing medium within the diffusion regime parametrised by the transport mean-free path l^*

$$-D_e \nabla^2 P_d(r, r_0) = \delta(r - r_0) \quad (2.6)$$

where $D_e = cl^*/d$ is the diffusion constant, d is the dimensionality of the problem ($d = 2$ for 2D and $d = 3$ for 3D), l^* is the transport mean-free path, r_0 the source position and c the transport velocity.

The diffuse intensity $P_d(r, r_0)$ will not be used for estimating l^* . Instead, the evolution of the diffusive transmission upon S matrix cascading will be used. This is because the ensemble averaging of wave intensity inside the disordered medium is computationally expensive.

The first half of the following section discusses the method by which spatially correlated disorders can be generated. The second half of the section connects the spatial correlation properties with that of the coherent mean-field, eventually leading to the estimation of l using the S matrix cascading method.

2.3 Coherent transmission, spatially correlated disorders and scattering mean-free path (l)

Ensembles of disorders can be broadly classified into two categories based on their spatial correlation properties of refractive index fluctuations, namely the correlated and the uncorrelated (white-noise like) disorders. Although the uncorrelated disorders with very small correlation length l_c (approaching zero) are analytically and computationally easier to implement, most cases practically (especially biological media) involve a finite (non-zero) spatial correlation length.⁸ The spatial correlation function plays an important role in determining the transport properties of the scattering medium. If the random disorder ensemble (characterised by its refractive index as a function of space) drawn from a particular probability distribution is considered as a spatial random process, then

7: The notation $P_d(r, r_0)$ is used for the diffuse intensity, to denote the "probability" of diffusion (or sometimes referred to as the diffusion approximation to a "diffusion"), to follow the same system of nomenclature given by [17].

8: As an example, for various kinds of mouse tissues, spatial correlation length l_c ranges from $\approx 5\mu m$ to $\approx 10\mu m$ (Refer Table 1 of [25])

[25]: Schmitt et al. (1996), 'Turbulent nature of refractive-index variations in biological tissue'

according to the Wiener–Khinchin theorem, the randomness power spectrum[72] of the disorder can be estimated by the spatial Fourier transform of its correlation function. Therefore, to create a random disorder with a particular correlation length, either the spatial correlation function (in real space) or the randomness power spectrum (in the spatial Fourier space), could be used. As an example, [72] and [73] use the desired spatial correlation function to spatially convolve (smoothen) a white-noise disorder to convert it into a correlated disorder with the desired correlation length l_c . In the following section, the Fourier space method using the desired power spectrum to generate a correlated disorder (with a desired l_c) is given.

[72]: Izrailev et al. (2012), ‘Anomalous localization in low-dimensional systems with correlated disorder’

[73]: Brandstötter et al. (2019), ‘Shaping the branched flow of light through disordered media’

2.3.1 Spatial correlation function and randomness power spectrum

Let the disorder be characterised by its relative dielectric constant $\tilde{\epsilon}_r(r)$ as function of $r = (z, y)$ (as given in equation 1.32 and Figure 1.9 of Chapter 1.)

$$\tilde{\epsilon}_r(r) = \tilde{\epsilon}_r^{ref} + \delta\tilde{\epsilon}_r(r) \quad (2.7)$$

In this chapter, the spatial perturbation $\delta\tilde{\epsilon}_r(r)$ has zero mean and has a uniform distribution. $\tilde{\epsilon}_r^{ref}$ corresponds to the dielectric constant of the reference (average background) medium upon which the spatial perturbation gets added and subtracted. In order to make the distance units used dimensionless, let the spatial lengths be given in terms of $k_{ref}z$ and $k_{ref}y$. To control the spatial texture of the disorder, a spatial correlation function has to be defined. For that, first define the following moments⁹ of the disorder perturbation

$$mean_{disorder} := \langle \delta\tilde{\epsilon}_r(k_{ref}z, k_{ref}y) \rangle = E(\delta\tilde{\epsilon}_r(k_{ref}z, k_{ref}y)) = 0 \quad (2.8)$$

$$\begin{aligned} var_{disorder} &:= \langle \delta\tilde{\epsilon}_r(k_{ref}z, k_{ref}y)^2 \rangle - \langle \delta\tilde{\epsilon}_r(k_{ref}z, k_{ref}y) \rangle^2 \\ &= \langle \delta\tilde{\epsilon}_r(k_{ref}z, k_{ref}y)^2 \rangle \end{aligned} \quad (2.9)$$

$$\begin{aligned} correlation_{disorder} &:= R(k_{ref}r, k_{ref}r_0) \\ &:= \langle \delta\tilde{\epsilon}_r(k_{ref}z, k_{ref}y) \delta\tilde{\epsilon}_r(k_{ref}z_0, k_{ref}y_0) \rangle \end{aligned} \quad (2.10)$$

where $correlation_{disorder} := R(k_{ref}r, k_{ref}r_0)$ is the un-normalised spatial correlation function. For a statistically homogeneous disorder, $R(k_{ref}r, k_{ref}r_0) = R(k_{ref}|r - r_0|)$. It can be noted from the definitions of the moments that $R(k_{ref}r_0, k_{ref}r_0) = R(0) = var_{disorder}$. Therefore, to represent the un-normalised spatial correlation function of the disorder, $R(0)$ value can be combined with a normalised¹⁰ correlation function $C_{disorder}(k_{ref}|r - r_0|)$ as given below

9: The angular bracket denotes the expectation operator acting on a random variable. If the ensemble of disorder is taken as a stationary random process, then the moments estimated by spatial averaging of one given disorder can be considered as an estimate for the ensemble averaged moments.

10: Note that the Gaussian correlation function is normalised such that $C_{disorder}(0) = 1$.

Disorder spatial correlation function

$$\begin{aligned} correlation_{disorder} &:= R(k_{ref}|r - r_0|) \\ &= R(0)C_{disorder}(k_{ref}|r - r_0|) \\ &= var_{disorder}C_{disorder}(k_{ref}|r - r_0|), \end{aligned} \quad (2.11)$$

where the normalised two-point Gaussian spatial correlation function for $\delta\tilde{\epsilon}_r(r)$ is given as the following.

$$C_{disorder}(k_{ref}|r - r_0|) = e^{-(k_{ref}|r-r_0|)^2/(k_{ref}l_c)^2} = e^{-|r-r_0|^2/l_c^2} \quad (2.12)$$

As said before, the power spectral density $P_{PSD}(p_z, p_y)$ of the disorder (considered as a spatial random process) is defined as the Fourier transform¹¹ of the correlation function $R(k_{ref}|r - r_0|) = R(0)C_{disorder}(k_{ref}|r - r_0|)$.

$$P_{PSD}(p_z, p_y) = \mathcal{F}\{R(k_{ref}|r - r_0|)\} = var_{disorder}\mathcal{F}\{C_{disorder}(r, l_c)\} \quad (2.13)$$

where p_z and p_y are angular spatial frequencies. The Fourier transform $\mathcal{F}\{C_{disorder}(r, l_c)\}$ can be evaluated using the equation 2.12 to obtain the final form¹² of $P_{PSD}(p_z, p_y)$

$$\begin{aligned} P_{PSD}(p_z, p_y) &= var_{disorder}\mathcal{F}\{C_{disorder}(r, l_c)\} \\ &= var_{disorder}\pi l_c^2 e^{-\frac{1}{4}l_c^2(p_y^2 + p_z^2)} \\ &= var_{disorder}\frac{\pi}{(1/l_c^2)} e^{-\frac{1}{4}\left(\frac{p_y^2 + p_z^2}{1/l_c^2}\right)} \end{aligned} \quad (2.14)$$

Next, the steps taken to create a uniformly distributed disorder with a given spatial correlation length l_c or randomness power spectrum $P_{PSD}(p_z, p_y)$, are given. Once the disorders are estimated, the attenuation of the mean-field is estimated to determine l . If $\epsilon_r^{white}(z, y)$ is the white noise disorder, then a uniformly-distributed spatially-correlated disorder $\epsilon_r^{corr}(z, y)$ can be generated from the white-noise disorder in two main steps. First, the white-noise disorder¹³ is convolved by the Gaussian correlation function. Such an operation results in a Gaussian-distributed correlated disorder and not a uniformly distributed one. Hence, to make the disorder uniformly distributed,¹⁴ a second step is needed. It involves a transformation method using a Gaussian cumulative probability distribution function. These two steps are explained as given below and the final results of the steps are given in Figure 2.2. As the convolution operation in real space is a product in the spatial Fourier space, the uniformly distributed correlated disorder can be estimated using the following steps.

1. Estimate $\delta\epsilon_{fft}^{white} = \text{fft2}(\delta\epsilon_r^{white}(z, y))$ where fft2 is the two dimensional fast Fourier transform.
2. Take an element-wise product in the Fourier space to obtain $\delta\epsilon_{fft}^{corr} = \delta\epsilon_{fft}^{white}\mathcal{F}\{C_{disorder}(r, l_c)\}$
3. Apply inverse Fourier transform to estimate the correlated disorder in the real space with spatial correlation length l_c

11: The spatial Fourier transform is defined as $\mathcal{F}\{f(z, y)\} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(z, y)e^{-i(zp_z + yp_y)} dz dy$.

12: A sanity check could be applied to the final form of P_{PSD} involving Parseval's theorem to see that $\frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} P_{PSD}(p_z, p_y) dp_z dp_y = R(0) = var_{disorder}$. The disorder randomness power spectrum $P_{PSD}(p_z, p_y)$ takes a Gaussian form and becomes broader when $1/l_c^2$ becomes larger or l_c becomes smaller. When $l_c \rightarrow 0$, the $P_{PSD}(p_z, p_y)$ becomes very broad (called as a white spectrum) and the sample in the real space becomes uncorrelated. Thus, the disorder power spectrum $P_{PSD}(p_z, p_y)$ determines the scattering potential of the disorder and thereby its scattering mean free path (l).

13: The White-noise disorder $\epsilon_r^{white}(z, y)$ can be easily generated in Matlab using the *rand* function generating a matrix of uniformly distributed random numbers. Such a disorder can be referred to as a Uniform white-noise disorder as the histogram of the matrix elements corresponds to a uniform probability distribution. The word "white" refers to the fact that the white noise disorders have their spatial correlation length $l_c \rightarrow 0$ or in other words they have flat power spectrum containing uniformly distributed power in the Fourier domain. On the other hand, if the histogram of the matrix elements of the disorder was Gaussian and its $l_c \rightarrow 0$, then the disorder is referred to as the Gaussian white-noise disorder.

14: A uniformly distributed disorder would scatter the waves better compared to a Gaussian distribution, for a given peak dielectric constant perturbation value within the disorder.

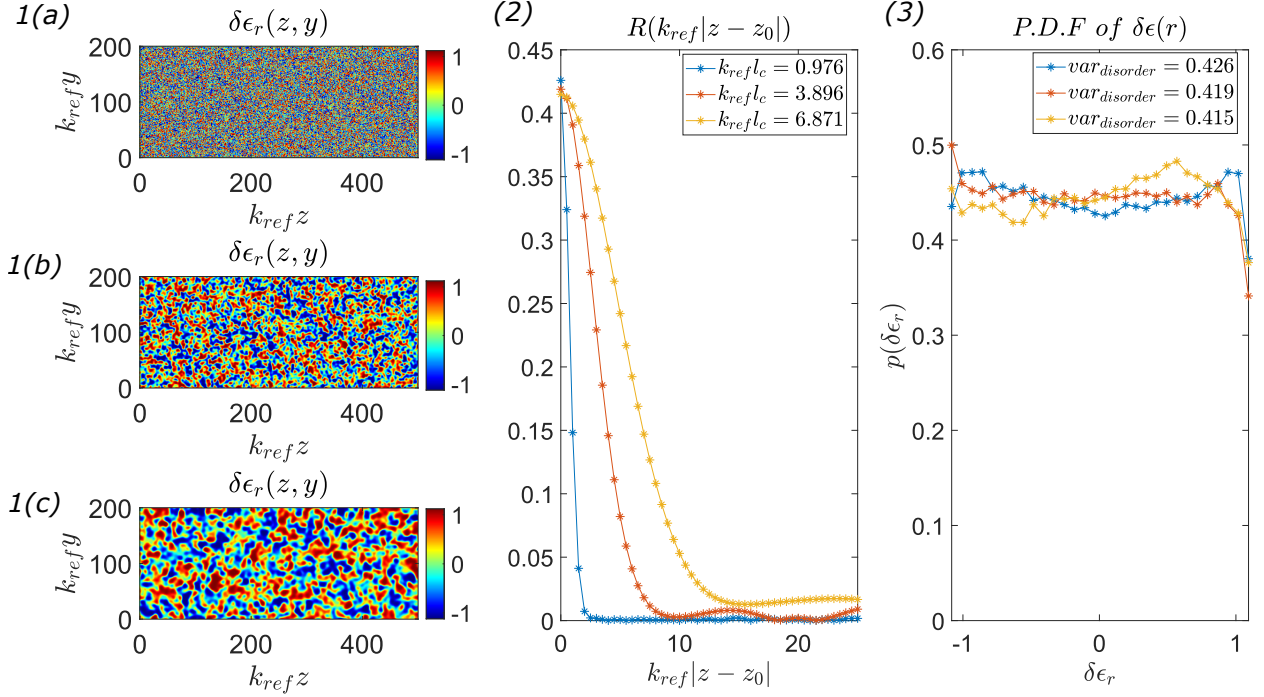


Figure 2.2: Examples to show the effects of spatial correlation on the disorder perturbation $\delta\epsilon_r(z, y)$. **1(a)** Uniformly distributed, Gaussian correlated disorders with $k_{ref}l_c = 0.976$, **1(b)** with $k_{ref}l_c = 3.896$ and **1(c)** with $k_{ref}l_c = 6.871$. The three disorder perturbations are represented on a grid with the same grid resolution such that $k_{ref}\Delta z = k_{ref}\Delta y = k_{ref}\Delta = 0.5$, which should be less than $k_{ref}l_c$ value taken. The uniformly distributed, Gaussian correlated disorders are obtained from the white noise disorder by the spatial Fourier method presented in Section 2.3.1. **(2)** The Correlation function $R_{disorder}(|k_{ref}(r - r_0)|)$ of the three samples shown in 1(a), 1(b) and 1(c). $R_{disorder}(0)$ corresponds to the variance of the disorder matrix elements as explained in the Section 2.3.1. **(3)** All the three disorders shown in 1(a), 1(b) and 1(c), are uniformly distributed disorders in the sense that the histogram of the disorder matrix elements (with grid size $k_{ref}\Delta = 0.5$) follow a uniform probability distribution with the nearly-same standard deviation of the white-noise disorder used to generate the correlated disorders.

$\delta\epsilon_r^{corr}(z, y) = \text{ifft2}(\delta\epsilon_{fft}^{corr})$ where ifft2 is the two dimensional inverse fast Fourier transform.

4. Normalise $\delta\epsilon_r^{corr}(z, y)$ by dividing it with the standard deviation of the matrix elements. This results in a Gaussian distributed (with unit variance) and Gaussian correlated (with correlation length l_c) disorder.
5. To transform the Gaussian distributed-Gaussian correlated disorder to a uniform distributed-Gaussian correlated disorder, a Gaussian cumulative probability distribution function (C.D.F) can be used. A zero mean Gaussian C.D.F takes a normally distributed random variable and converts it into a transformed random variable between (0, 1) giving a uniform distribution. Hence, every matrix element of Gaussian distributed-Gaussian correlated disorder can be transformed between (0, 1) using the Gaussian C.D.F. Such a uniformly distributed disorder between (0, 1) can then be scaled between $(\min(\delta\epsilon^{white}), \max(\delta\epsilon^{white}))$, to have similar spread in values with that of the uncorrelated white-noise disorder.
6. The real space spatial correlation of the obtained disorder can be numerically estimated and validated against the l_c value used for defining the correlation function by the following method. It involves the Fourier space method for evaluating the spatial autocorrelation of a 2D matrix. For an $M \times N$ correlated disorder $\delta\epsilon_r^{corr}(z, y)$, $R_{disorder}(k_{ref}|r - r_0|) = |\text{ifft2}(\text{fft2}(\delta\epsilon_r^{corr})\text{conj}(\text{fft2}(\delta\epsilon_r^{corr})))|/(M * N)$

where conj denotes complex conjugation. The numerically estimated correlation length can be defined as the length at which the correlation function decays from $R(0)$ to $R(0)/e$.

Results of these steps are plotted in Figure 2.2 showing examples for uniformly distributed correlated disorders with different spatial correlation lengths l_c .¹⁵

2.3.2 Generating spatially correlated and uncorrelated disorders using cascading method

As defined in the equation 2.3, the scattering mean free path (l) is defined with respect to the attenuation of the statistically coherent mean-field associated with ensemble averaging of the sample. For ensemble averaging, the transmission matrices of an ensemble of samples has to be estimated. Such an estimation of a larger number of thick samples could be computationally tedious. A work-around would be the cascading method discussed in Section 1.8 of Chapter 1. S matrices for a collection of thin samples can be estimated for once and these thin layers can be cascaded to obtain an effective S matrix for a thicker sample. The effective S matrices for an ensemble of thick samples can be obtained by shuffling the order of cascading of the thinner slabs. The spatial correlation length l_c determines the thickness of the thin slabs used for cascading. As l_c can also be interpreted as the spatial “memory” associated with the random sample, thinner slabs with longitudinal thickness L_{slice} larger than at least 5 correlation lengths ($L_{\text{slice}} > 5l_c$) would be very dissimilar to each other.

2.3.3 Coherent mean-field attenuation, l and the generalised Reynold’s number for correlated disorders

As hinted before, the spatial correlation length l_c and the randomness power spectrum, determines the scattering mean-free path l of the disorder and it is manifested as the attenuation of the coherent mean-field. The attenuation of the coherent mean-field is parameterised¹⁶ by the combination of l_c and $R_{\text{disorder}}(0)$, given by a dimensionless number called as the generalised Reynold’s number¹⁷ $R_e = (k_{\text{ref}} l_c)^2 \text{var}_{\text{disorder}}$. For a given finite $\text{var}_{\text{disorder}}$, $R_e \ll 1$ (with comparatively small $\text{var}_{\text{disorder}}$) indicates weaker scattering by the sample. On the other hand when R_e is larger than the order of unity (implying l_c of the order of wavelengths λ , with not-so-small $\text{var}_{\text{disorder}}$) causes strong multiple scattering.

Steps for estimating the scattering mean free path (l) for spatially correlated disorders

1. First, generate an ensemble of S matrices involving p number of thinner disorders with a given correlation length l_c and $\text{var}_{\text{disorder}}$, with a thickness of $L_{\text{slice}} \geq 5l_c$.¹⁸ To estimate the transport behaviour only due to diffusive multiple scattering, it is better if the sample is placed in a refractive index matched background medium

15: The steps used to transform a uniformly-distributed white-noise disorder to a uniformly distributed correlated disorder can be interpreted as an effective clustering operation performed on the white-noise disorder matrix elements, to group the matrix elements containing similar dielectric constant values to form larger particle aggregates.

16: For more details and the proof on how the mean-field is dependent on the spatial correlation, refer to the Appendix Section A.12.

17: Refer equation number 4.62 of [30].

[30]: Frish (1968), ‘Wave propagation in random media’

18: For generating correlated slabs, refer to the details given in Section 2.3.1 and Section 2.3.2. For the cascading method involving scattering matrices, Section 1.8 of Chapter 1 may be referred.

so that the specular reflectance is minimised. Next, S matrices are cascaded by growing the sample thickness one slice at a time.

2. Estimate S_{21} by cascading the S matrices of thinner layers and observe the evolution of the S_{21} as a function of total sample thickness L (along z) of the cascaded thicker slab, which is an integer multiple of the thickness of the thinner slab slice.
3. Estimate an ensemble average $\langle S_{21} \rangle$ at every cascading step, to bring out the statistically coherent mean-field component of the transmission matrix. Such an ensemble averaging can be easily performed by shuffling the order of the cascading of the S matrices of the thinner slab slices. Estimate the coherent mean-field transmission as a function of length L , $\tau_{coherent}(L) = \frac{1}{M} \text{Trace} \{ \langle S_{21} \rangle^\dagger \langle S_{21} \rangle \}$, where M is the number of input modes. This step is similar in essence with that of the method given in [63] and [74] in which uncorrelated disorders were used.
4. Estimate the $1/e$ extinction length (which is the scattering mean free path l) at which the coherent transmission becomes $1/e$, by fitting an attenuating exponential function.

Before getting into the numerical estimation of l associated with the coherent transmission, the diffusion theory involving the classically incoherent (diffusive) transmission is reviewed in the next section for estimating the transport mean-free path (l^*).

2.4 Statistically incoherent wave-field, diffusion theory and transport mean free path (l^*)

In this section, the standard diffusion theory is reviewed followed by the estimation of the l^* for the correlated disorders.

2.4.1 A review of the analytical diffusion theory using spatial Fourier transform

The steady-state diffusion equation for a non-absorbing medium is given as the following

Steady-state diffusion equation for a non-absorbing medium

$$-D_e \nabla^2 P_d(r, r_0) = \delta(r - r_0), \quad (2.15)$$

where $D_e = cl^*/d$ is the diffusion constant, d is the dimensionality of the problem ($d = 2$ for 2D and $d = 3$ for 3D), l^* is the transport mean-free path and r_0 , the source position. Here, the solution $P_d(r, r_0)$ within the context of quantum transport is known as the probability of diffusion (also called as the diffusion approximation of the “diffuson”¹⁹) at the position r , associated with a diffusive source injected at the position r_0 . For solving the diffusion equation analytically, boundary conditions are needed to be defined along the transverse dimension (along y for the 2D problem) and the longitudinal (along z) dimension of the slab medium. Solving

[63]: Shi et al. (2018), ‘Diffusion in translucent media’

[74]: Yilmaz et al. (2019), ‘Transverse localization of transmission eigenchannels’

19: Refer chapter 5 of Akkermans and Montambaux[17]. The steady state diffusion equation (equation 2.15) has also been widely used for solving the heat diffusion problem and hence a vast collection of analytical solutions[75] exists for the diffusion equation under various geometries.

[75]: Carslaw et al. (1992), *Conduction of heat in solids*

the diffusion equation analytically for a slab medium ($W \gg L$) gets considerably simplified, if an infinitely extending slab geometry along the transverse dimension (along y) is taken so that the translational invariance of the solution with respect to y_0 of the source location is obtained. Therefore, in 2D, $P_d(z, z_0, y, y_0) = P_d(z, z_0, y - y_0) = P_d(z, z_0, \rho)$, hence the y dependency of the solution depends only on the difference $\rho = y - y_0$. Then, the spatial Fourier transform along ρ could be used transform the problem into the spatial Fourier domain so that the variable ρ gets transformed into q . Hence, the solution $P_d(z, z_0, \rho)$ gets transformed into $P_d(z, z_0, q)$ in the spatial Fourier domain. Followed by the implementation of extrapolated (Robin boundary condition)²⁰ at $z = 0$ and $z = L$, the diffusion equation for the slab can be solved as given below. (For the analytical derivation in 2D solved using Mathematica, refer to Section A.13.)

$$P_d(z, z_0, q) = \begin{cases} P_d^+(z, z_0, q) & \text{if } z \geq z_0 \\ P_d^-(z, z_0, q) & \text{if } z < z_0 \end{cases} \quad (2.16)$$

$$P_d^+(z, z_0, q) = \frac{(ql^*z_e \cosh(qz_0) + \sinh(qz_0))(ql^*z_e \cosh(q(L-z)) + \sinh(q(L-z)))}{qD_e \left(\sinh(Lq) \left(q^2 l^{*2} z_e^2 + 1 \right) + 2ql^*z_e \cosh(Lq) \right)} \quad (2.17)$$

$$P_d^-(z, z_0, q) = \frac{(ql^*z_e \cosh(qz) + \sinh(qz))(ql^*z_e \cosh(q(L-z_0)) + \sinh(q(L-z_0)))}{qD_e \left(\sinh(Lq) \left(q^2 l^{*2} z_e^2 + 1 \right) + 2ql^*z_e \cosh(Lq) \right)} \quad (2.18)$$

where z_e is the dimensionless extrapolation boundary length ratio²¹ such that, $z_e l^*$ is the longitudinal size of the extrapolated boundary from the surface of the slab. Integrating the solutions, equation 2.17 and equation 2.18, with respect to the transverse dimension (along y in 2D or along x and y in 3D) at a given z value inside the slab, would yield the following 1D equations for $z \geq z_0$ and $z < z_0$ respectively.

$$\int_{-\infty}^{+\infty} P_d^+(z, z_0, y) dy = \lim_{q \rightarrow 0} P_d^+(z, z_0, q) = \frac{(l^*z_e + z_0)(l^*z_e + L - z)}{D_e(2l^*z_e + L)} \quad (2.19)$$

$$\int_{-\infty}^{+\infty} P_d^-(z, z_0, y) dy = \lim_{q \rightarrow 0} P_d^-(z, z_0, q) = \frac{(l^*z_e + z)(l^*z_e + L - z_0)}{D_e(2l^*z_e + L)} \quad (2.20)$$

where the limits were evaluated using Mathematica. These 1D equations (transverse integrated solutions) are the same, irrespective of the choice²² of the transverse boundary condition being either an insulating boundary or the slab infinitely extending along y . The total transmission T can be evaluated by integrating along y , the z component of the diffusion

20: The extrapolated or the Robin boundary condition in the diffusion theory is a partially absorbing boundary condition. It results in a linear attenuation of the P_d from the given z value at 0 or L until the extrapolated boundary placed at $z_e l^*$ from 0 or L , outside of the diffusive slab.

21: For a refractive index matched slab, $z_e = 2/3$ in 3D and $z_e = \pi/4$ in 2D[17]. On the other hand, if there is a refractive index mismatch between the sample and the surrounding medium, then the boundary effects for internal boundary scattering has to be incorporated for the diffusion theory. One may refer to[76] for more details on R . Then, in 3D, z_e becomes $z_e = (2/3) [(1+R)/(1-R)]$ where R is the angle integrated[76] internal Fresnel reflectance when diffusive wave propagates from the inside to the outside of the disorder.

22: It is possible to analytically solve the diffusion problem with transverse reflective boundary conditions, in terms of eigenfunction expansion of the solution. But, this will make the solution $P_d(z, z_0, q)$ a bit more detailed than the one used in the chapter. Transverse integration of the solution along y with the transverse insulating boundary conditions, would still provide the same results given in equation 2.19 and 2.20.

current $\vec{J}_d(z, y, \rho)$ crossing the boundaries at $z = L$. Similarly, the total reflection R from the slab can be evaluated by doing the same integration process at $z = 0$.

The diffusion current $\vec{J}_d(z, z_0, \rho)$ is defined by the Fick's first law as $\vec{J}_d(z, z_0, \rho) = -D_e \nabla P_d(z, z_0, \rho)$ and the z component of the diffusion current is $\vec{J}_d^{(z)}(z, z_0, \rho) = -D_e \frac{\partial}{\partial z} P_d(z, z_0, \rho)$. Hence, the total transmission and the reflection can be estimated using equation 2.19 and 2.20, as the following

$$\begin{aligned} T &= \int_{-\infty}^{+\infty} \vec{J}_d^{(z)}(z, z_0, \rho)|_{z=L} d\rho = \int_{-\infty}^{+\infty} \left\{ -D_e \frac{\partial}{\partial z} P_d^+(z, z_0, y) dy \right\} |_{z=L} \\ &= -D_e \frac{\partial}{\partial z} \left\{ \int_{-\infty}^{+\infty} P_d^+(z, z_0, y) dy \right\} |_{z=L} = \frac{l^* z_e + z_0}{L + 2l^* z_e} = \frac{z_e + \frac{z_0}{l^*}}{\frac{L}{l^*} + 2z_e} \quad (2.21) \end{aligned}$$

$$\begin{aligned} R &= - \int_{-\infty}^{+\infty} \vec{J}_d^{(z)}(z, z_0, \rho)|_{z=0} d\rho = \int_{-\infty}^{+\infty} \left\{ +D_e \frac{\partial}{\partial z} P_d^-(z, z_0, y) dy \right\} |_{z=0} \\ &= +D_e \frac{\partial}{\partial z} \left\{ \int_{-\infty}^{+\infty} P_d^-(z, z_0, y) dy \right\} |_{z=0} = \frac{l^* z_e + L - z_0}{L + 2l^* z_e} = \frac{z_e + \frac{L}{l^*} - \frac{z_0}{l^*}}{\frac{L}{l^*} + 2z_e} \quad (2.22) \end{aligned}$$

obtaining the well known result reported in [70, 77] for total transmission, where z_0 is taken as l^* . From the given expression for T and R , it could be easily verified that $R + T = 1$ and the flux conservation is obeyed. The dependence²³ of total transmission T on L and l^* , or the dependence of the transverse integrated P_d on L and l^* could be used to estimate the l^* from the wave transport modelling results to be discussed in the next main section.

Finite sized incident beam profile

For obtaining the solution $I_d(z, z_0, y, y_0)$ for a finite sized incident beam profile, the following convolution integral between $P_d(z, z_0, y, y_0)$ and the incident beam with transverse beam profile $F_{inc}(y)$, injected at $z = l^*$ can be used.

$$I_d(z, y) = \int_{-\infty}^{+\infty} F_{inc}(y_0) P_d(z, z_0 = l^*, y - y_0) dy_0 \quad (2.23)$$

where $F_{inc}(y_0)$ for different beam geometries, are given as the following

$$F_{inc}(y) = \begin{cases} \text{Gaussian beam profile} := \frac{1}{\sqrt{\pi} D_{in}} e^{-\frac{y^2}{D_{in}^2}} \\ \text{Rectangular beam profile} := \begin{cases} 1/D_{in} & \text{when } -D_{in}/2 < y < D_{in}/2 \\ 0 & \text{otherwise} \end{cases} \end{cases} \quad (2.24)$$

$F_{inc}(y)$ is normalised such that $\int_{-\infty}^{+\infty} F_{inc}(y) dy = 1$. As equation 2.23 is a convolution integral in real space, it turns to be a simple product in the spatial Fourier domain as shown below.

$$I_d(z, q) = F_{inc}(q) P_d(z, z_0 = l^*, q) \quad (2.25)$$

[77]: Li et al. (1993), 'Transmission and surface intensity profiles in random media'

[70]: Durian (1994), 'Influence of boundary reflection and refraction on diffusive photon transport'

23: If $L/l^* \gg 1$ and the source injection point z_0 is taken as l^* , then the total transmission can be approximated as $T = \left(z_e + \frac{z_0}{l^*} \right) / \left(\frac{L}{l^*} + 2z_e \right) \approx (z_e + 1) / (L/l^*) = \frac{5}{3} \frac{l^*}{L}$ where $z_e = 2/3$ for 3D and $T = \left(1 + \frac{\pi}{4} \right) (l^*/L)$ where $z_e = \pi/4$ for 2D.

where, the Fourier transform $F_{inc}(q)$ is given as the following

$$F_{inc}(q) = \begin{cases} \text{Gaussian beam profile} := e^{-\frac{1}{4}D_{in}^2 q^2} \\ \text{Rectangular beam profile} := \sin\left(\frac{qD_{in}}{2}\right) / \left(\frac{qD_{in}}{2}\right) \end{cases} \quad (2.26)$$

such that, $\lim_{q \rightarrow 0} F_{inc}(q) = 1$ due to the normalisation $\int_{-\infty}^{+\infty} F_{inc}(y) dy = 1$ as defined before. Therefore, the y integrated diffusion profile is given as

$$\begin{aligned} \int_{-\infty}^{+\infty} I_d(z, y) dy &= \lim_{q \rightarrow 0} I_d(z, q) \\ &= \lim_{q \rightarrow 0} F_{inc}(q) P_d(z, z_0 = l^*, q) \\ &= \lim_{q \rightarrow 0} P_d(z, z_0 = l^*, q) \\ (\because \lim_{q \rightarrow 0} F_{inc}(q) &= 1) \end{aligned} \quad (2.27)$$

where the product rule of limits is used, recovering the same 1D expressions given in equation for a point source at $z_0 = l^*$. Also, the expressions for T and R remains the same form.²⁴ This concludes the review of diffusion theory involving l^* . In the next section, this diffusion theory is compared against the transmission data obtained from the S matrix cascading to estimate l^* for the spatially correlated disorders.

2.4.2 Estimation of l and l^* from the S matrix cascading and the role played by spatial correlation

Steps for estimating transport mean free path (l^*)

1. Evaluate all the steps given before in Section 2.3.3 for estimating the scattering mean free path (l).
2. Estimate the ensemble averaged total transmission as a function of L , $\tau_{total}(L) = \langle \frac{1}{M} \text{Trace}\{S_{21}^\dagger S_{21}\} \rangle$ where M is the number of input modes. Note that this ensemble averaging is different from the one given in step 3 of the Section 2.3.3 for estimating l . Here, the ensemble averaging of total transmission is done after evaluating the trace of $S_{21}^\dagger S_{21}$. In the step 3 of the Section 2.3.3, first the ensemble averaging is performed on the S_{21} matrix (not on the transmission) and then the coherent transmission is estimated by applying the trace formula.
3. Compare $\tau_{total}(L)$ with that of the analytically known equation for transmission (equation 2.21) and estimate l^* . The exact steps taken to compare and obtain the l^* is given in the side note.²⁵

The estimation of l and l^* is performed for two different regimes of disorder randomness. The first regime is the case when the generalised Reynold's number $R_e = (k_{ref} l_c)^2 \text{var}_{disorder}$ is smaller than the order of unity and the second regime is when R_e is larger than the order of unity. For different disorders with varying randomness properties to be categorised into the first or the second regime, the l and l^* are estimated. Using the methods explained in Section 2.3.3, l is estimated by fitting an exponential function with an attenuation length of l . Also, the l^* is estimated from the $1/T$ plot as described in this section.

24: Hence, the analytical forms of the equations for T and R for a slab medium, are independent of the incident beam profile when the beam profile is normalised as $\int_{-\infty}^{+\infty} F_{inc}(y) dy = 1$.

25: Steps for estimating l^* from equation 2.21 is given below. Let z_0/l^* be called as z_p , the injection depth ratio, which is a dimensionless term indicating the relative penetration depth at which the diffusion source is placed. Then, equation 2.21 can be re-written as

Transmission and inverse transmission

$$T = \frac{z_e l^* + z_p l^*}{L + 2z_e l^*} \quad (2.28)$$

$$\frac{1}{T} = \left(\frac{1}{(z_e + z_p) l^*} \right) L + \left(\frac{2z_e}{z_p + z_e} \right) \quad (2.29)$$

For a YX plot of $1/T$ vs L , the y intercept extrapolated at $L = 0$ can be obtained as

$$\frac{1}{T}|_{L=0} = \frac{2z_e}{z_p + z_e} \quad (2.30)$$

Similarly, the x intercept extrapolated at $(1/T) = 0$ is given as

$$L|_{(1/T)=0} = -2z_e l^* \quad (2.31)$$

First, z_e is estimated as given before in a side note within the Section 2.4.1. Then, the x intercept $L|_{(1/T)=0}$ is estimated by extrapolating the data obtained from the modelling, by fitting a straight line^[77] onto the $1/T$ data. From these values, l^* is estimated as per equation 2.31. Similarly, using equation 2.30, z_p is estimated as the y intercept and z_e value are known. Such a method of estimating l^* is followed in many papers such as [63, 77, 78].

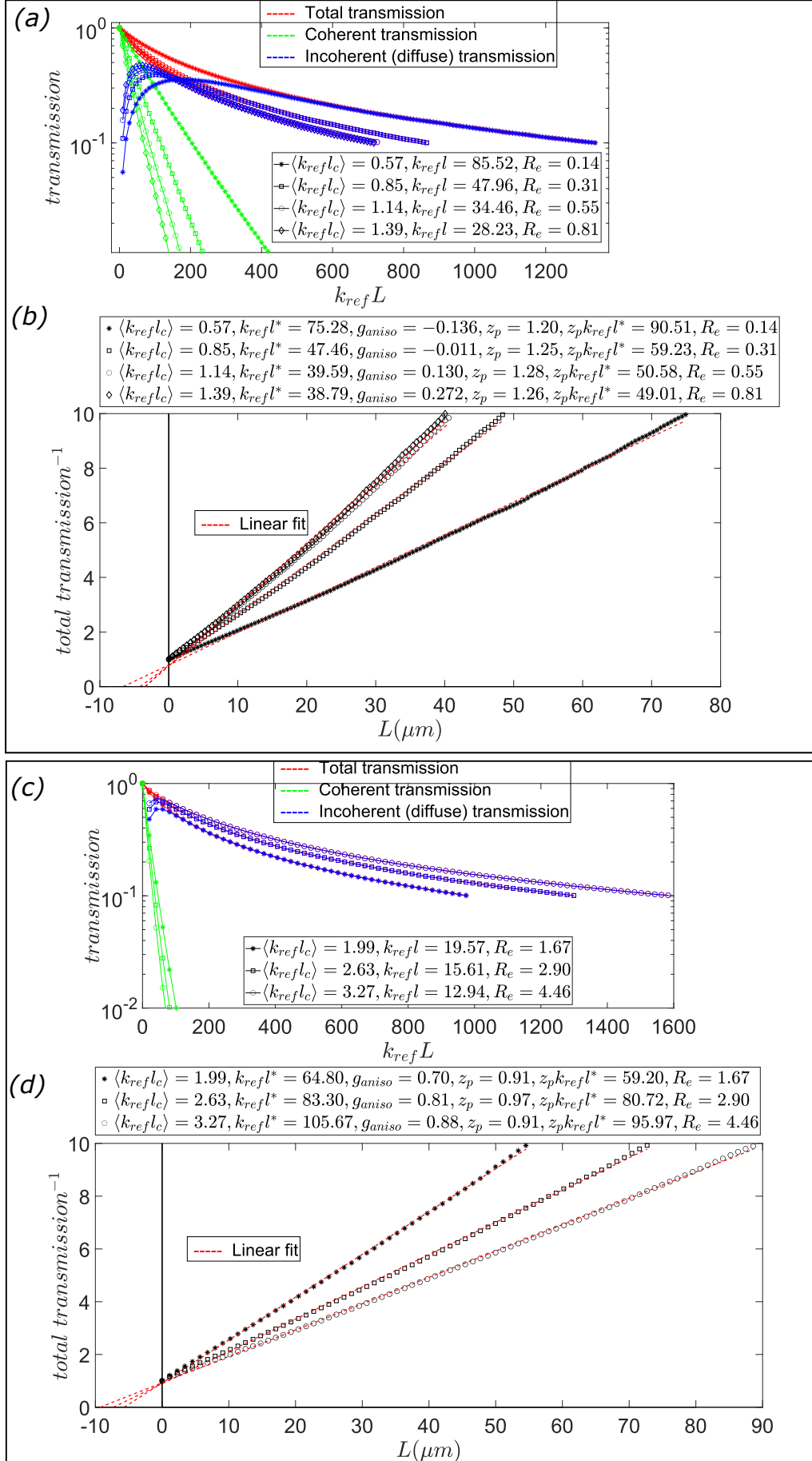


Figure 2.3: Plotting the wave transport transmission data obtained from the S matrix cascading and the role played by the generalised Reynold's number, $R_e = \left(k_{ref} l_c\right)^2 var_{disorder}$. Plots (a) and (b) are for the scenario where $R_e < 1$ which could be referred to as comparatively weak scattering. On the other hand, for (c) and (d) the $R_e > 1$ and the regime of operation is now within the strong scattering regime. When $R_e < 1$, it can be seen that when $k_{ref} l_c$ increases, l^* decreases and saturates. Such a trend reverses when $R_e > 1$, where l^* increases when $k_{ref} l_c$ increases. l decreases consistently when $k_{ref} l_c$ increases for both regimes.

The trends associated with different kinds of transmissions with respect to increase in $k_{ref}L$ (associated with the S matrix cascading) are shown in Figure 2.3.

When the generalised Reynold's number, R_e , is smaller than the order of 1.

- ▶ As shown in the Figure 2.3(a) and (b), when R_e is comparatively smaller when compared to the order of 1, an increase in $k_{ref}l_c$ results in the decrease of the dimensionless scattering mean-free path $k_{ref}l$.
- ▶ In addition, the anisotropy g_{aniso} starts to increase (from a nearly isotropic scattering to partially anisotropic) and also the dimensionless transport mean-free path $k_{ref}l^*$ first decreases and then saturates.
- ▶ Along with that, the total transmission of the slab after completing the cascading process, also decreases first and then saturates upon increasing the $k_{ref}l_c$ value.

When R_e is larger than the order of 1.

- ▶ The trend for $k_{ref}l^*$ reverses for R_e larger than the order of unity as shown in the Figure 2.3(d), as when $k_{ref}l_c$ increases $k_{ref}l^*$ also increases.
- ▶ It can also be seen that the anisotropy also increases (from partially anisotropic to highly anisotropic) when $k_{ref}l_c$ increases.
- ▶ Along with that, the total transmission of the slab after completing the cascading process, increases upon increasing the $k_{ref}l_c$ value.
- ▶ Such a reversal of the trend for $k_{ref}l^*$ and total transmission, with respect to increase in $k_{ref}l_c$ when changing the regime of scattering from small R_e value to large R_e value, occurs mainly because of the increase in anisotropy, from regime of nearly isotropic to largely anisotropic scattering. Such an increase in spatial correlation causes the scatters to be forward scattering thereby increasing the transmission and also increasing the l^* value.

Until now, diffusion theory involving a slab geometry was discussed. For arbitrary geometries (for example, having an insulating aperture inside the disorder), the analytical way of solving the problem could lead to complicated and lengthier analytical expressions involving Fourier series summation. Instead, for simplicity²⁶ the Finite Difference Time domain (FDTD) formulation of the diffusion equation can be employed. In the next subsection, the FDTD formulation of the diffusion problem is discussed.

26: First order formulation of the diffusion equation, involving Fick's law and the diffusion current, can be used to tailor and design the diffusive flow for arbitrary geometries. The FDTD method estimates the temporal impulse response of diffusive pulse source and upon integrating the impulse response in time, the steady-state response can be estimated.

2.4.3 FDTD formulation of the diffusion equation for tailored geometries

This section describes the finite difference time domain (FDTD) formulation of the diffusion equation as a coupled set of first order derivatives involving $P_d(z, z_0, y, y_0, t)$ and the diffusion current vector field $\vec{J}(z, z_0, y, y_0, t)$, forming a continuity equation (involving a staggered grid structure). Such a formulation is particularly helpful in this chapter

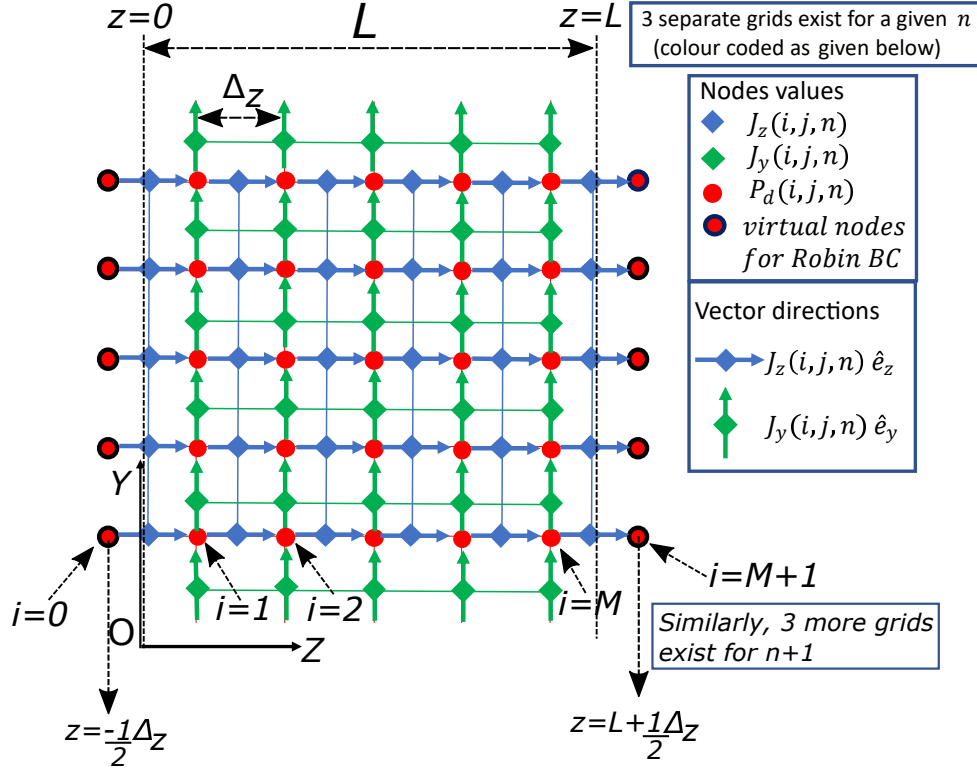


Figure 2.4: Staggered grid system used for the FDTD diffusion formulation for arbitrary geometries. n denotes the n^{th} time-step and (i, j) are index variables for the grid nodes. For a given n , there are 3 separate grids existing in the computational memory, namely $P_d(i, j, n)$, $J_z(i, j, n)$, and $J_y(i, j, n)$ placed in a staggered arrangement as shown in the figure. In addition to the 3 grids, there is also a grid for $P_d(i, j, n+1)$ at the $(n+1)^{\text{th}}$ step. Each grid has its own local coordinate system indexed by the same notation (i, j, n) , avoiding the use of a global notation system applicable of all the grids together. A forward difference scheme is adopted for discretising both the temporal and spatial derivative operators. $J_z(i, j, n)$ or $J_y(i, j, n)$ could be set to zero while time stepping for defining insulating boundaries, preventing the diffusion current along z and y respectively. For implementing the Robin boundary condition at $z = 0$ and $z = L$, virtual nodes are needed as shown.

for defining insulated surfaces (preventing diffusion through them) and constricted channels, by explicitly setting the z or y current components in $\vec{J}(z, z_0, y, y_0, t)$ to zero²⁷ in the numerical implementation while time stepping. Diffusive response function of a spatio-temporal Dirac-delta impulse function within the medium can be recorded using the FDTD method. The steady-state response by a continuous source could then be modelled by the temporal integration of the impulse response function from $t = 0$ to $t = \infty$ (theoretically) or to a large time value (numerically). Consider the following time domain diffusion equation in 2D as an initial value problem

27: In the diffusion theory, setting $P_d(z, y, t)$ to zero at a spatial location while time stepping is an absorbing boundary condition (not an insulating one). For the insulating boundary condition, the current component J_z or J_y has to be set to zero. On the other hand, for wave transport modelling, setting the field to zero while time stepping is a reflecting(mirror) boundary condition.

Time domain diffusion equation

$$\left[\frac{\partial}{\partial t} - D_e \nabla^2 \right] P_d(z, y, t) = 0 \quad (2.32)$$

with an initial condition of $P_d(z, y, t = 0) = \delta(z - z_0)\delta(y - y_0)$ and two kinds of boundary conditions. The first kind of boundary condition is the insulating boundary condition placed for insulating surfaces, especially at the transverse boundaries and also at any other surfaces restricting the diffusion process. The second kind is the Robin boundary condition at

$z = 0$ and $z = L$, as given in equations A.162 and A.163. D_e is assumed to be uniform within the computational domain. The equation 2.32 having second order spatial derivatives and a first order temporal derivative, is split into two first order equations involving $P_d(z, z_0, y, y_0, t)$ and $\vec{J}(z, z_0, y, y_0, t)$, forming a continuity equation as given below

$$\begin{aligned} \frac{\partial}{\partial t} P_d(z, y, t) &= - \left[\frac{\partial}{\partial z} \left(-D_e \frac{\partial}{\partial z} \right) + \frac{\partial}{\partial y} \left(-D_e \frac{\partial}{\partial y} \right) \right] P_d(z, y, t) \\ &= - \left[\hat{e}_z \frac{\partial}{\partial z} + \hat{e}_y \frac{\partial}{\partial y} \right] \cdot \left[\underbrace{\left(-D_e \frac{\partial}{\partial z} P_d(z, y, t) \right)}_{J_z(z, y, t)} \hat{e}_z + \underbrace{\left(-D_e \frac{\partial}{\partial y} P_d(z, y, t) \right)}_{J_y(z, y, t)} \hat{e}_y \right] \\ &= -\nabla \cdot \vec{J}(z, y, t) \end{aligned} \quad (2.33)$$

where $\cdot$ is the notation for the dot product and $\hat{e}_z$ and $\hat{e}_y$ are the unit vectors along z and y . $\vec{J}(z, y, t) = J_z(z, y, t)\hat{e}_z + J_y(z, y, t)\hat{e}_y$ is the diffusion current vector field. $J_z(z, y, t)$ or $J_y(z, y, t)$, could be set to zero at the desired grid nodes (z, y) to create insulated regions preventing diffusion current flow along the directions $\hat{e}_z$ and $\hat{e}_y$ respectively. The continuity equation is discretised on a staggered grid system described in Figure 2.4. For such a discretisation scheme, let n denote the index for the time step, i for the z locations and j for the y locations. The Fick's first law can then be discretised (dropping the d from P_d for convenience in representation) as

$$J_{i,j,n}^y = -D_e \left(\frac{1}{\Delta_y} \right) (P_{i,j+1}^n - P_{i,j}^n) \quad (2.34)$$

$$J_{i,j,n}^z = -D_e \left(\frac{1}{\Delta_z} \right) (P_{i+1,j}^n - P_{i,j}^n) \quad (2.35)$$

followed by the discretisation of Fick's second law given in equation 2.33 to obtain

$$\frac{1}{\Delta_t} (P_{i,j}^{n+1} - P_{i,j}^n) = -\frac{1}{\Delta_z} (J_{i+1,j}^{z,n} - J_{i,j}^{z,n}) + -\frac{1}{\Delta_y} (J_{i,j+1}^{y,n} - J_{i,j}^{y,n}) \quad (2.36)$$

The time stepping scheme can then be implemented by solving for $P_{i,j}^{n+1}$ from the above equation as given below

$$P_{i,j}^{n+1} = P_{i,j}^n - \frac{\Delta_t}{\Delta_z} (J_{i+1,j}^{z,n} - J_{i,j}^{z,n}) + -\frac{\Delta_t}{\Delta_y} (J_{i,j+1}^{y,n} - J_{i,j}^{y,n}) \quad (2.37)$$

with a Dirac-delta initial condition $P_{i=j_0}^{n=0} = 1/(\Delta_z \Delta_y)$ at $t = 0$ (hence, a Dirac-delta in time and space) in the given location (i_0, j_0) . The Robin boundary condition at the left and the right slab surfaces ($z = 0$ and $z = L$ with respect to the slab thickness L), can be discretised as the following. The discretisation involves the virtual nodes outside the slab region L as shown in Figure 2.4. Let the z position index of the virtual nodes on the left side of the slab be denoted as $\frac{-1}{2}\Delta_z$ which is half a cell from $z = 0$ and one grid cell left to the interior $P_{i=1,j}^n$ point as shown in

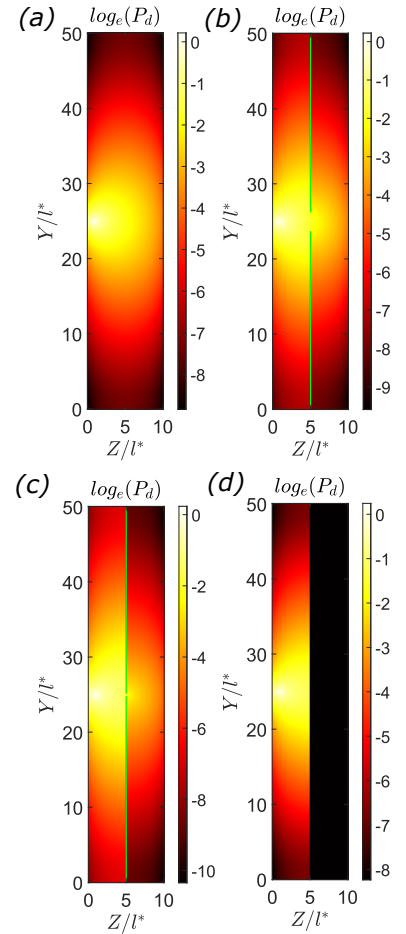


Figure 2.5: Diffusion probability for various slab geometries involving an insulating aperture are shown. The plots are estimated using the FDTD diffusion method given in Section 2.4.3. . Logarithm of the probability of diffusion P_d is plotted for a medium (a) with no aperture present where $T = 0.149979, R = 0.850017, T + R = 0.999996$ for the slab with $L = 10l^*$ and $W = 50l^*$, (b) when an insulating aperture (shown as a Green line) with a dimensionless opening width of $W/D_{in} = 20$ where $T = 0.095436, R = 0.904560, T + R = 0.999996$, (c) when $W/D_{in} = 150$ such that $T = 0.046207, R = 0.953789, T + R = 0.999997$ and finally (d) when the aperture is fully closed and completely insulating.

the Figure 2.4. Similarly, on the right side of the slab, let the virtual nodes have an z position index denoted by $L + \frac{1}{2}\Delta_z$, as it is half cell right to the slab surface at L . To implement the Robin boundary condition on the left and the right surface of the slab, the $P_{i,j,n}$ values has to be evaluated precisely at the left and the right surface. It is estimated by averaging the virtual nodes and the interior nodes as given below, due to the reason that there are no P_d nodes defined at the left and right slab surfaces. Using a mixed notation²⁸ for purpose of intuitive representation as given below

$$P_{z=0,j}^n = \frac{1}{2} \left(P_{z=-\frac{1}{2}\Delta_z,j}^n + P_{i=1,j}^n \right) = \frac{1}{2} \left(P_{i=0,j}^n + P_{i=1,j}^n \right) \quad (2.38)$$

$$P_{z=L,j}^n = \frac{1}{2} \left(P_{z=L+\frac{1}{2}\Delta_z,j}^n + P_{z=L,j}^n \right) = \frac{1}{2} \left(P_{i=M+1,j}^n + P_{i=M,j}^n \right) \quad (2.39)$$

Then, the Robin boundary conditions can be implemented as the following using which the z component of the diffusion current is estimated at the left and right surface of the slab shown in the Figure 2.4. The Robin boundary condition given in equations A.162 and A.163, can be discretised as the following. At the left surface (at $z = 0$ with respect to the slab)

$$P(z, y, t)|_{z=0} - z_e l^* \frac{\partial}{\partial z} P(z, y, t)|_{z=0} = 0 \implies -\frac{D_e}{l^* z_e} P(z=0, y, t) = -D_e \frac{\partial}{\partial z} P(z, y, t)|_{z=0} = J^z(z, y, t)|_{z=0} \quad (2.40)$$

Using equation 2.38, the z component of the diffusion current at the left surface of the slab can be estimated as

$$J_{z=0,j,n}^z = -\left(\frac{D_e}{l^* z_e} \right) \frac{1}{2} (P_{i=0,j} + P_{i=1,j}) \quad (2.41)$$

Similarly, the z component of the diffusion current at the right surface of the slab can be estimated as the following

$$\begin{aligned} J_{z=L,j,n}^z &= \left(\frac{D_e}{l^* z_e} \right) \frac{1}{2} \left(P_{z=L+\frac{1}{2}\Delta_z,j} + P_{z=L-\frac{1}{2}\Delta_z,j} \right) \\ &= \left(\frac{D_e}{l^* z_e} \right) \frac{1}{2} (P_{i=M+1,j} + P_{i=M,j}) \end{aligned} \quad (2.42)$$

During the time stepping process, the virtual nodes can be updated using the conventional Fick's law for the diffusion current. Using equation 2.35

$$P_{z=L+\frac{1}{2}\Delta_z,j}^n = P_{z=L-\frac{1}{2}\Delta_z,j}^n + \left(\frac{-\Delta_z}{D_e} \right) J_{z=L,j,n}^z \quad (2.43)$$

$$P_{z=-\frac{1}{2}\Delta_z,j}^n = P_{i=1,j}^n + \left(\frac{\Delta_z}{D_e} \right) J_{z=0,j,n}^z \quad (2.44)$$

To summarise, the *FDTD* algorithm is given in the sidenote.²⁹ For the stable operation of the time stepping *FDTD* time stepping algorithm, the parameters involved, namely D_e , Δ_t , Δ_z & Δ_y have to obey the following

28: Mixed notation implies mixing the indices such as i with the space coordinate z . To avoid confusion, alternate representations involving only the indices are also provided.

29: *FDTD* algorithm :
Initialise all the grid arrays shown in Figure 2.4, to be zero.

- **Step 1** : At $t = 0$, initialise the pulsed source as a spatio-temporal Dirac-delta function at (i_0, j_0) , $P_{i=i_0,j=j_0}^{n=0} = 1/(\Delta_z \Delta_y)$.
- **Step 2** : Estimate diffusion currents at the interior $P_d(i, j, n)$ nodes (using equations 2.34 and 2.35). Also, estimate diffusion currents at the virtual $P_d(i, j, n)$ nodes, outside of the the region L using equations 2.41 and 2.42.
- **Step 3** : Set the current flow boundary conditions at insulating locations by initialising $J_{i,j}^{z,n}$ or $J_{i,j}^{y,n}$ to zero, depending upon the direction of flow which needs to be prevented at a certain (i, j) location.
- **Step 4** : Estimate $P_{i,j}^{n+1}$ in the interior nodes using the equation 2.37. Also estimate $P_{z=-\frac{1}{2}\Delta_z,j}^n$ and $P_{z=L+\frac{1}{2}\Delta_z,j}^n$ at the virtual nodes using the equations 2.43 and 2.44.
- **Step 5** : Update the grid $P_{i,j}^n = P_{i,j}^{n+1}$. Accumulatively add (integrate) and store on a grid, the response $P_{i,j}^n$ at every time step to estimate the steady state response. Repeat the steps 1 to 5 until the pulse energy has exited out the medium.

stability³⁰ condition [79]

$$D_e \Delta_t \left(\frac{1}{(\Delta_z)^2} + \frac{1}{(\Delta_y)^2} \right) < \frac{1}{2} \quad (2.45)$$

The diffusion *FDTD* modelling examples involving an insulating aperture with an orifice placed on the middle of a slab of thickness $L = 10l^*$ are shown in Figure 2.5. In the next section, the total transmission scaling law in terms of two parameters, namely the L/l^* ratio and the injection depth ratio z_p , is discussed. The *FDTD* diffusion method described in this section would also be used to validate the transmission scaling law.

30: The stability condition ensures that Δ_t has to be small enough such that the speed by which the diffusion time-steps on the grid, should be less than the actual physical transport velocity c by which the diffusion would have propagated in reality.

2.5 Total transmission scaling law involving S matrix cascading, analytical diffusion theory and the diffusion *FDTD* method

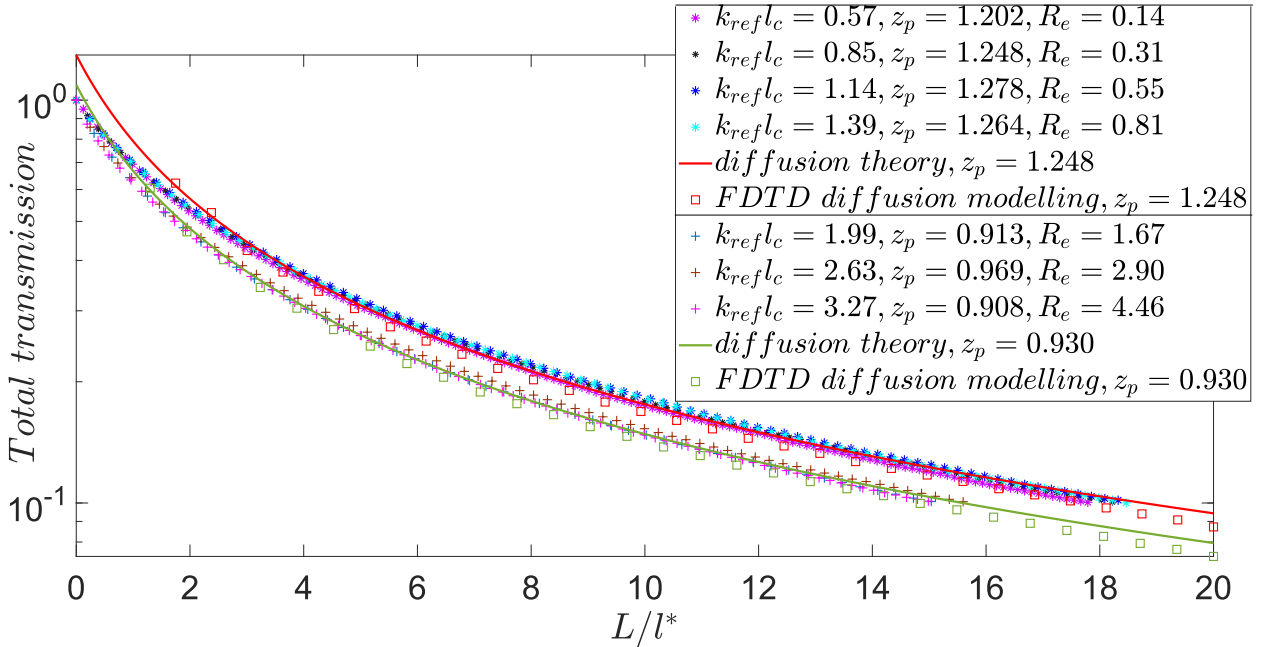


Figure 2.6: Validation of the two parameter total transmission scaling law, involving 1) S matrix cascading obtained from the wave transport theory for spatially correlated disorders, 2) analytical diffusion theory using spatial Fourier transform and 3) the numerical *FDTD* method for the diffusion, is shown. The total transmission scaling law given in equation 2.46 involves two parameters, namely the L/l^* ratio and the injection depth ratio z_p , as a function of the spatial correlation length and the Reynold's parameter R_e . All the data obtained nearly falls on the same transmission scaling law. Two separate instances of the same transmission scaling law are shown because for smaller R_e value, averaged $z_p = 1.248$ and for the larger R_e value, averaged $z_p = 0.930$.

Upon reading this thesis, the reader may notice the following two aspects regarding the modelling frameworks presented. The first aspect is that in all the transport models, the total transmission and reflection fluxes are conserved such that $T + R = 1$. The second aspect is that, relatively smaller samples are modelled when compared to the size of the typical samples used for the experimental scenario. One could ask the question whether using such small samples is in any way restrictive to the comprehension of the underlying physics of the transport phenomena. Computationally efficient modelling of wave transport for larger disorder ensembles

involving millions of scattering particles, is a research topic by itself, which is not the aim and scope of this thesis. The aim and scope of this thesis is to explore a collection of wave transport phenomena, with the limited computational capacity available. Hence, the longitudinal size of the slab can be represented in terms of dimensionless term L/l^* and reflecting transverse boundary can be used to preserve flux conservation. Therefore, different combinations of L and l^* , giving same L/l^* value and same injection depth ratio of z_p , would yield same kind of transmission trend with respect to L , irrespective of the number of scatterers being ten thousand or ten million. Best way to check such an assertion is to compare the total transmission data given in Figure 2.3 obtained using the S matrix cascading (which used a relatively small sample) against the expression for the total transmission³¹ given by the analytical diffusion theory and the numerical method of diffusion $FDTD$ given in Section 2.4.3. The diffusion theory generally accommodates larger macroscopic media. Figure 2.6 demonstrates the transmission scaling law.

2.6 Conclusion

In this chapter, the statistical characterisation of the disorder randomness in terms of spatial correlation, together with the cascading and ensemble averaging involving S matrices, is used to link the scattering properties. These scattering properties include the scattering mean-free path, transport mean-free path and scattering anisotropy, described as a function of the disorder spatial correlation and randomness. Such a study will be useful for designing disorders with the desired transport properties. Coherent wave scattering and classically incoherent diffusion theory are compared side by side, to discuss the similarities involved in the theories which address the same transport phenomena. The two parameter transmission scaling law is verified for disorders with different randomness properties. It implies that one could implement wave scattering models obeying flux conservation with comparatively smaller samples, to predict the transmission and the reflection behaviour of large macroscopic slabs.

31: From equation 2.28, the transmission scaling law is given as,

Transmission scaling law

$$T = \frac{z_p + z_e}{(L/l^*) + 2z_e} \quad (2.46)$$

The methods in the Time Domain for wavefront shaping

3

3.1 Introduction

This chapter introduces the methods used for solving the scalar Helmholtz equation in the time domain using the Finite Difference Time Domain (*FDTD*) scheme. The time domain methods are explored in this chapter as opposed to the frequency domain methods given in Chapter 1, mainly to model two time-dependent phenomena. They are the Space-Time Modulation (*STM*) and the effect of sample decorrelation due to the Brownian motion, in the context of wavefront shaping. Space-time modulation (a practical example being the acousto-optic effect) is an important phenomenon to consider. That is because the *STM* has the potential to form an acousto-optic “guide-star”[4, 26, 27] by which waves could be wavefront-shaped to focus inside random media. The effect of sample decorrelation on wavefront shaping[80] is also a relevant phenomenon to study as dynamical media such as tissue, scrambles the transmitted wavefront (as a function of time) due to random internal scatterer motion. An overview of the *FDTD* schemes presented in the chapter, mainly to study space-time modulation and sample decorrelation, is provided using three separate figures given in Figure 3.1, Figure 3.2 and Figure 3.3.

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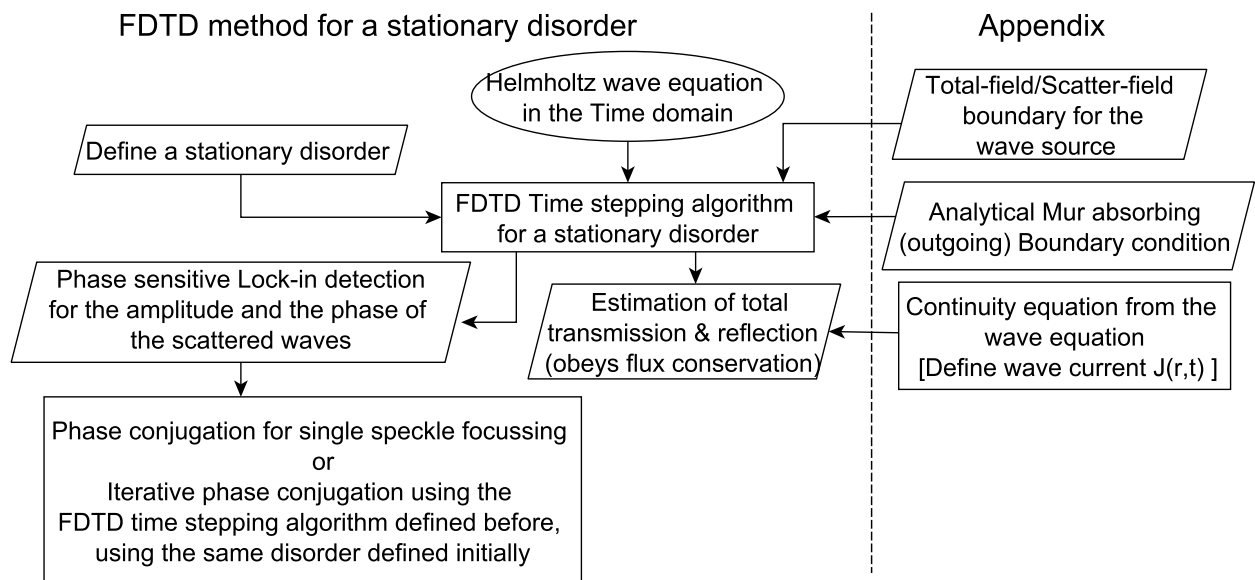


Figure 3.1: The overview of the *FDTD* formulation, involving a stationary disorder and the associated wavefront shaping applications, is shown. For the details on the implementation, refer Section 3.2 and Section 3.3. A total-field/scatter-field boundary is placed on the source side to separate out the reflected wave from the incident wave. At the transmitted and the reflected detection boundaries, a phase-sensitive lock-in detection (*PSD*) scheme is implemented to estimate the amplitude and phase of the outgoing wave. Upon knowing the amplitude and phase of the transmitted wavefront, one could create a phase conjugate version of the wave set as an array of dipole sources on the detection boundary. Such a phase conjugate wave partially overcomes the conventional multiple scattering phenomena and focusses back to the original dipole source location.

Figure 3.1, Figure 3.3 and Figure 3.2, correspond to the *FDTD* methods

associated with a stationary medium, a medium containing a Space-Time modulated (STM) region and a decorrelating medium with Brownian motion, respectively.¹ Some of the basic elements in the time-domain method (such as the boundary conditions, the estimation of total transmission and reflection etc..) recur between the three flow charts. The

1: Modelling these time-dependent phenomena would otherwise be a harder problem (computationally and analytically) in the frequency domain and hence the presentation of the time-domain methods in this chapter.

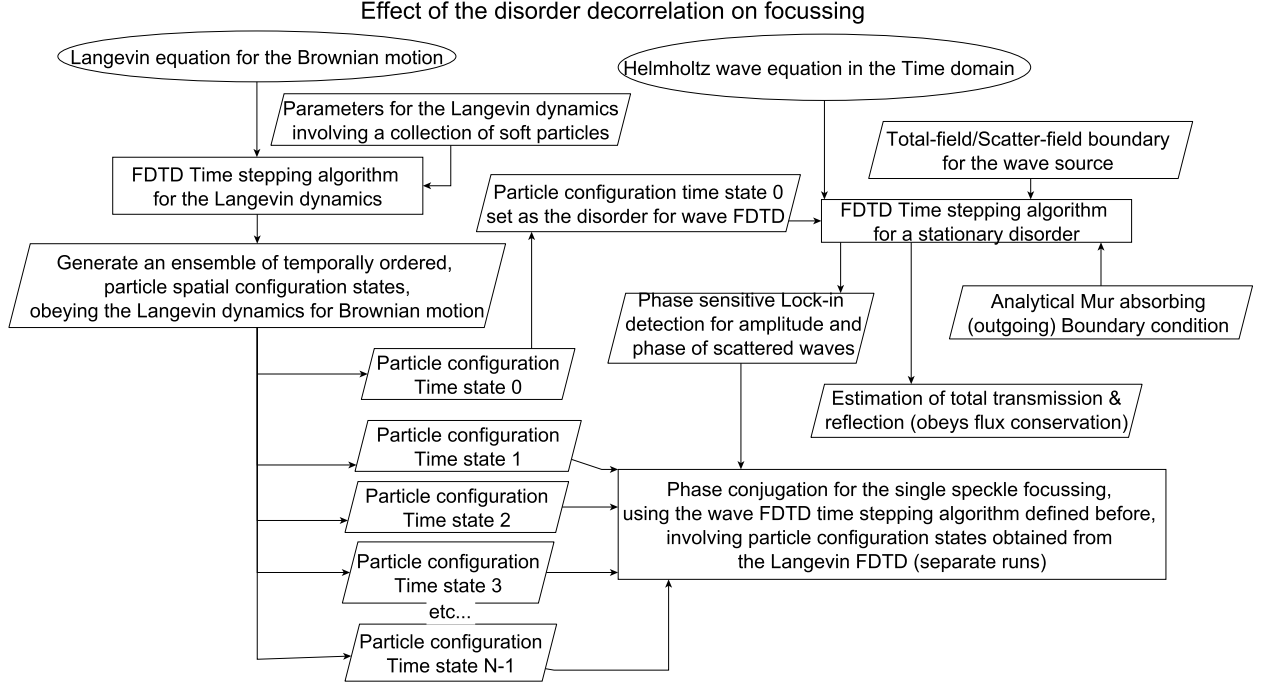


Figure 3.2: Overview of the FDTD formulation, involving a Brownian decorrelating medium and the associated wavefront shaping application, is shown. The quasi-static approximation is incorporated such that, separate wave FDTD runs using the obtained disorder spatial configuration states from the Langevin equation is performed. In other words, the random media doesn't evolve continuously according to the Langevin equation while performing the wave FDTD time-stepping. Instead, the wave transport steady-state is achieved in separate/individual runs using stationary particle configuration states taken one at a time.

important and the relevant details on the computational implementation of these methods will be discussed in the chapter. For the finer details, the developed Matlab codes associated with the FDTD methods given in the chapter can be referred. For maintaining the conciseness of the chapter, flowcharts given in Figure 3.1, Figure 3.2 and Figure 3.3 are not discussed separately one after the other. Instead, the important ideas will be discussed in the relevant sections of the chapter and a diligent reader can easily contextualise these ideas with respect to the presented flowcharts.

Towards the beginning of the chapter, the FDTD formulation for a stationary disorder is provided as summarised by Figure 3.1. It also discusses the methods to estimate the amplitude and phase of the transmitted wavefront² and the method by which, one could estimate the total transmission and reflection, by integrating the wave current crossing the relevant boundaries. Once the phase conjugate (PC) wave is defined,³ the PC wave could be used for single speckle focussing (for high contrast focussing) or iterative optical phase conjugation (for enhancement of total transmission).

Once the phase conjugate wave is obtained forming a focus back at the original dipole source location, the decorrelation effects of this focal spot with respect to Brownian motion is studied⁴ using the FDTD

2: Such an estimation of the amplitude and phase of the scattered wave, is valuable for defining a phase conjugate wave to be used for focussing back overcoming the conventional multiple scattering.

3: Phase conjugate wave can be defined by setting $t = -t$ (or $\omega_0 = -\omega_0$) dependence on the measured amplitude and phase of the forward-going scattered wave and injecting the phase conjugate wave at the same spatial location from which the wave amplitude and phase were measured.

4: For the study involving the decorrelation effects on the wavefront shaped focal spot, two kinds of FDTD time stepping are involved. First is the FDTD time stepping performed on the Langevin equation for Brownian motion. Second is the familiar FDTD time stepping method for the Helmholtz equation, already summarised in Figure 3.1.

FDTD method involving a Space-Time modulated (STM) region

Appendix

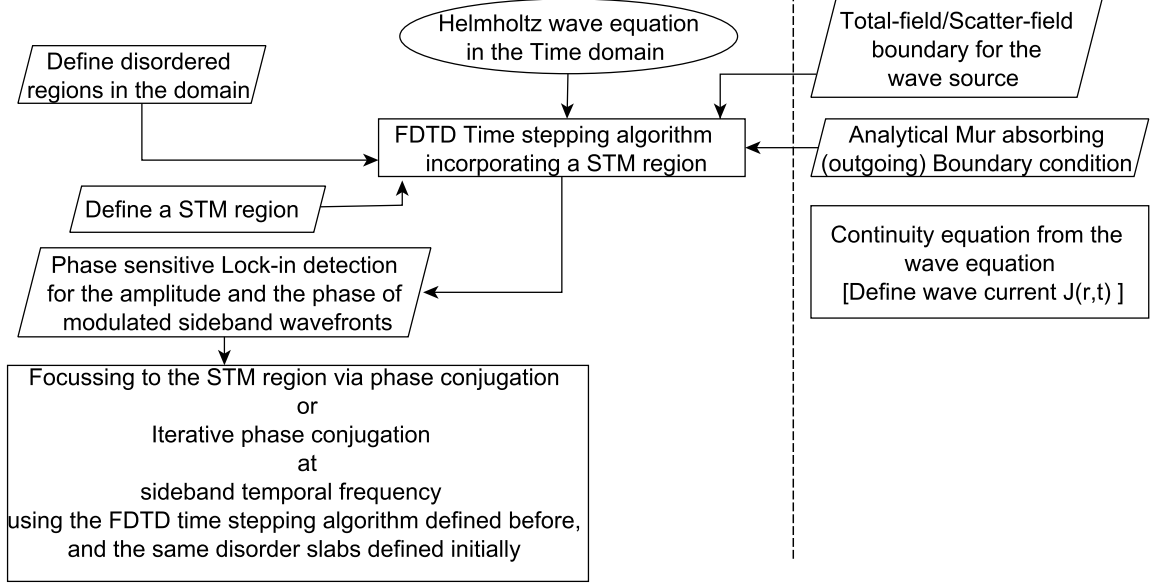


Figure 3.3: Overview of the *FDTD* formulation, involving a space-time modulated (STM) region and the associated wavefront shaping application, is shown. For details on the implementation, refer to Section 3.5. Incident light gets multiple-scattered by the disorder and gets spatially and temporally modulated by the *STM* region. A phase-sensitive lock-in detection scheme is implemented to estimate the amplitude and phase of the transmitted modulated sideband at $\omega_0 + \omega_{mod}$ where ω_0 is the carrier-light temporal angular frequency and ω_0 the *STM* temporal modulation angular frequency. Detected sideband wavefront is phase-conjugated at $\omega_0 + \omega_{mod}$ which focuses back to the *STM* region.

formulation of the Langevin equation for Brownian motion. The *FDTD* time stepping framework, involving the Langevin equation and the Helmholtz equation, is summarised in Figure 3.2.

Finally, towards the last portion of the chapter, the wavefront shaping *FDTD* formulation in presence of a *STM* guide-star⁵ is presented (Refer Figure 3.3 for an overview). In the following section, a second order⁶ *FDTD* formulation of the Helmholtz wave equation in the time domain is given.

3.2 Finite difference Time domain (*FDTD*) formulation of the wave equation for a stationary random medium

The Helmholtz wave equation in time domain (refer equation 4.3 of [81] or equation 19 of [82]) with time dependent dielectric constant ($\epsilon_r(r, t)$) is given as

Generalised Time-domain Helmholtz wave equation

$$\nabla^2 E(r, t) - \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} (\epsilon_r(r, t) E(r, t)) = 0, \quad (3.1)$$

5: *FDTD* formulation for the stationary disorder can be obtained by setting the *STM* modulation to be zero, both in space and time.

6: This chapter presents the discretised form of the second order Helmholtz equation containing the second order spatial and temporal derivatives. The second order temporal derivative is a necessity with respect to the time reversal invariance property of the solution to the Helmholtz wave equation in non-absorbing media. On the other hand, the diffusion equation presented in chapter 2, which contains a first order temporal derivative, has no time reversal invariance property. Hence, it is recommended **not** to time-reverse the trajectory of a Monte Carlo photon computationally, which is based on light diffusion in general, lacking time reversal invariance property physics-wise.

[81]: Korpel (1972), 'Acousto-optics'

[82]: Taravati et al. (2019), 'Generalized space-time-periodic diffraction gratings: Theory and applications'

where $E(r, t)$ is the real valued wave field, $\epsilon_r(r, t)$ is the time dependent relative dielectric permittivity constant, c_0 is the free space light wave velocity and the relative permeability constant is assumed to be unity. In this section, the *FDTD* formulation for the stationary disorder is considered and hence the dielectric permittivity constant $\epsilon_r(r, t)$ is taken independent⁷ of time so that $\epsilon_r(r, t) = \epsilon_r(r)$. Therefore,

Time-domain Helmholtz wave equation for a stationary disorder

$$\nabla^2 E(r, t) - \frac{\epsilon_r(r)}{c_0^2} \frac{\partial^2}{\partial t^2} E(r, t) = 0 \quad (3.2)$$

Discretising equation 3.2 using the second order central difference scheme (refer section 2.4 of [32] or [83]), the following is obtained for a 2D problem

$$\frac{E(y, z + \Delta_z, t) - 2E(y, z, t) + E(y, z - \Delta_z, t)}{\Delta_z^2} + \frac{E(y + \Delta_y, z, t) - 2E(y, z, t) + E(y - \Delta_y, z, t)}{\Delta_y^2} = \epsilon_r(y, z) \left[\frac{E(y, z, t + \Delta_t) - 2E(y, z, t) + E(y, z, t - \Delta_t)}{(c_0 \Delta_t)^2} \right], \quad (3.3)$$

where Δ_z and Δ_y are the discrete grid size elements along z and y respectively. On a discrete grid, let z, y and t be indexed⁸ by the variables i, j and n such that $z = (i - 1)\Delta_z, y = (j - 1)\Delta_y$ and $t = (n - 1)\Delta_t$, where $i, j, n \in (1, 2, 3, 4, \dots)$. Therefore, the equation 3.3 is rewritten as

$$\frac{E_{i+1,j}^n - 2E_{i,j}^n + E_{i-1,j}^n}{\Delta_z^2} + \frac{E_{i,j+1}^n - 2E_{i,j}^n + E_{i,j-1}^n}{\Delta_y^2} = \epsilon_{r,i,j} \left[\frac{E_{i,j}^{n+1} - 2E_{i,j}^n + E_{i,j}^{n-1}}{(c_0 \Delta_t)^2} \right] \quad (3.4)$$

For further simplification, let $\Delta_z = \Delta_y = \Delta_s$. Then, equation 3.4 is given as

$$\left(E_{i+1,j}^n - 2E_{i,j}^n + E_{i-1,j}^n \right) + \left(E_{i,j+1}^n - 2E_{i,j}^n + E_{i,j-1}^n \right) = \frac{\epsilon_{r,i,j} \Delta_s^2}{(c_0 \Delta_t)^2} \left[E_{i,j}^{n+1} - 2E_{i,j}^n + E_{i,j}^{n-1} \right] \quad (3.5)$$

Defining a factor $w_0 = (\epsilon_{r,i,j} \Delta_s^2) / ((c_0 \Delta_t)^2)$ appearing in the *R.H.S* of the above equation and rearranging⁹ the equation to solve for $E_{i,j}^{n+1}$, the following is obtained.

FDTD time stepping equation for a stationary medium in 2D

$$E_{i,j}^{n+1} = 2E_{i,j}^n - E_{i,j}^{n-1} + \frac{1}{w_0} \left[\left(E_{i+1,j}^n - 2E_{i,j}^n + E_{i-1,j}^n \right) + \left(E_{i,j+1}^n - 2E_{i,j}^n + E_{i,j-1}^n \right) \right] \quad (3.6)$$

7: *FDTD* formulation for a time dependent $\epsilon_r(r, t)$ will be discussed later in the chapter, in Section 3.5.

[32]: Taflove et al. (2005), *Computational electrodynamics: the finite-difference time-domain method*

[83]: Toroglu et al. (2014), 'Finite-difference time-domain (fdtd) matlab codes for first-and second-order EM differential equations [testing ourselves]'

8: Summary of indices :

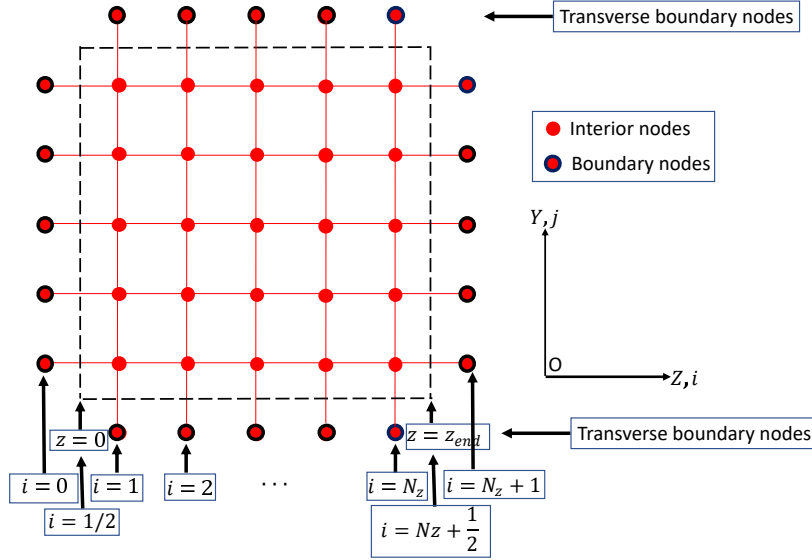
- z indexed by i such that $z = (i - 1)\Delta_z$
- y indexed by j such that $y = (j - 1)\Delta_y$
- time t is indexed by n , such that $t = (n - 1)\Delta_t$

where $i, j, n \in (1, 2, 3, 4, \dots)$. On the contrary, on a 2D Matlab grid, z position is accessed by the column and y position accessed by the row. In other words, if E^n is a grid in Matlab, then the notation $E_{i,j}^n$ given in the chapter, is stored and accessed in Matlab as $E^n(j, i)$, where the order of (j, i) is reversed compared to (i, j) .

9: Rearranging the equation is to obtain the wave field $E_{i,j}^{n+1}$ at the future time step $n + 1$, in terms of the current state of the wave field $E_{i,j}^n$ at the time step n and the past field $E_{i,j}^{n-1}$ at the time step $n - 1$.

The time stepping equation given in equation 3.6 could be used to uniquely determine the wave field evolution upon providing the suitable boundary conditions. Next subsection explains the implementation of the boundary conditions.

3.2.1 Implementation of boundary conditions



10: Analytic ABCs are incorporated along z axis boundaries and reflecting (mirror) boundaries are implemented at the transverse boundaries. This is to simplify the estimation of transmission and reflection, only at two surfaces. If the outgoing boundary condition is implemented at the transverse boundaries, then four surfaces are needed to be taken care of to estimate the total transmission and the reflection from the disorder.

Figure 3.4: Schematic for explaining the boundary condition.

Two kinds of boundary conditions are employed in this chapter. The first kind is the reflecting (mirror) boundary condition which could be easily implemented in the *FDTD* routine by setting the $E_{i,j}^n = 0$ at the desired boundary position at all time values. In this chapter, the transverse boundary condition at $y = 0$ and $y = W$, is set to be the reflecting boundary condition. The second kind of boundary condition implemented is at the longitudinal boundary planes at $z = 0$ and $z = z_{end}$, to cause the scattered waves to be outgoing waves.¹⁰ Such a kind of boundary condition, called as the Absorbing boundary condition (ABC), is implemented so that the transmitted and the reflected waves from the disorder propagate outwards from the longitudinal grid z boundaries without being reflected back. Two main kinds of ABC exists, namely the Perfectly Matched Layer (PML) boundary conditions and the analytic ABC.¹¹ PML boundary conditions are superior to Analytic ABCs with respect to boundary reflections, but the former requires somewhat cumbersome formulations especially via analytic continuation^[85] of the space variables into the complex domain, significantly altering the simple form of the time stepping equation given in equation 3.6. Hence, for simplicity, the generalisation to the second order Mur ABC¹² are used and such an ABC is sufficient for the kind of applications intended in this chapter. At $z = 0$,

$$\frac{\partial^2 E(r, t)}{\partial z \partial t} - \frac{p_0}{c_{ref}} \frac{\partial^2 E(r, t)}{\partial t^2} + p_2 c_{ref} \frac{\partial^2 E(r, t)}{\partial y^2} = 0 \quad (3.7)$$

At $z = z_{end}$,

$$\frac{\partial^2 E(r, t)}{\partial z \partial t} + \frac{p_0}{c_{ref}} \frac{\partial^2 E(r, t)}{\partial t^2} - p_2 c_{ref} \frac{\partial^2 E(r, t)}{\partial y^2} = 0 \quad (3.8)$$

11: For a historical review of various forms of absorbing boundary conditions, refer to [84]

[84]: Bérenger (2015), 'A historical review of the absorbing boundary conditions for electromagnetics'

[85]: Johnson (2008), 'Notes on perfectly matched layers (PMLs)'

12: Refer section 6.3.3, "Trefethen-Halpern Generalized and Higher-Order ABCs" of [32] for details

where in the ‘‘Chebyshev on a subinterval’’ approximation[32], $p_0 = 1.00023$ and $p_2 = 0.51555$. Also, $c_{ref} = c_0/\sqrt{\epsilon_{ref}}$, where ϵ_{ref} is the average dielectric constant of the reference(background) medium. The discrete forms of the equations 3.7 and 3.8 for time stepping at the boundaries are given as the following. (The derivations for the discrete form of the analytical absorbing boundary conditions, given in equations 3.7 and 3.8, are given in the Section A.14.)

Discrete form of the analytical absorbing boundary condition

At $z = 0$,

$$E_{0,j}^{n+1} = -E_{1,j}^{n-1} + \frac{c_{ref}\Delta t - p_0\Delta z}{c_{ref}\Delta t + p_0\Delta z} \left(E_{0,j}^{n-1} + E_{1,j}^{n+1} \right) + \frac{2p_0\Delta z}{c_{ref}\Delta t + p_0\Delta z} \left(E_{0,j}^n + E_{1,j}^n \right) + \frac{p_2 c_{ref}^2 \Delta t^2 \Delta z}{\Delta_y^2 (c_{ref}\Delta t + p_0\Delta z)} \left\{ \left(E_{0,j-1}^n + E_{0,j+1}^n - 2E_{0,j}^n \right) + \left(E_{1,j-1}^n + E_{1,j+1}^n - 2E_{1,j}^n \right) \right\} \quad (3.9)$$

At $z = z_{end}$,

$$E_{N_z+1,j}^{n+1} = -E_{N_z,j}^{n-1} + \frac{c_{ref}\Delta t - p_0\Delta z}{c_{ref}\Delta t + p_0\Delta z} \left(E_{N_z+1,j}^{n-1} + E_{N_z,j}^{n+1} \right) + \frac{2p_0\Delta z}{c_{ref}\Delta t + p_0\Delta z} \left(E_{N_z+1,j}^n + E_{N_z,j}^n \right) + \frac{p_2 c_{ref}^2 \Delta t^2 \Delta z}{\Delta_y^2 (c_{ref}\Delta t + p_0\Delta z)} \left\{ \left(E_{N_z+1,j-1}^n + E_{N_z+1,j+1}^n - 2E_{N_z+1,j}^n \right) + \left(E_{N_z,j-1}^n + E_{N_z,j+1}^n - 2E_{N_z,j}^n \right) \right\} \quad (3.10)$$

In addition to these outgoing boundary conditions, there is also a Total-Field/Scatter-Field(TF/SF) [53] boundary condition used for separating out the reflected wave from the total wave due to an incident wave source in the computational domain. Such a formulation of the boundary condition is essential for the estimation and visualisation of the back reflected scattered wave from the sample, without getting mixed with the source wave. Next subsection explains how total transmission and reflection is estimated from the scattered waves.¹³

3.2.2 Estimation of total transmission and reflection in FDTD formulation

The estimation of the total transmission (T) and total reflection (R) for a non-absorbing medium, is based on the definition of the wave current density $\vec{J}(r, t)$ estimated at the detection boundaries Γ_R and Γ_L respectively, as shown in the Figure 3.5. Once $\vec{J}(r, t)$ is evaluated at the detection boundaries, where T and R are evaluated respectively, the z component of $\vec{J}(r, t)$ normal to the detection boundary can be estimated. Integrating the z component of the wave current density for one wave temporal cycle, followed by a spatial integration along the boundary (along y), yields the net wave current (flux) crossing the boundary. The expression for the wave current density $\vec{J}(r, t)$ is obtained from the continuity equation associated with the Helmholtz equation in the time domain, as derived in the Appendix Section A.15. The local form of

[53]: Umashankar et al. (1982), ‘A novel method to analyze electromagnetic scattering of complex objects’

13: The estimation of the total transmission (T) and reflection (R), by integration of the wave current at the relevant boundaries, is given in the Section 3.2.2. Such an estimation has the following advantages.

- Estimation of the T and R in a non-absorbing medium serves as a safety test to check whether the FDTD code implementation works as intended. This is because, by the conservation of wave flux, $R + T = 1$.
- T serves as scalable parameter with respect to L/l^* and other physical parameters under consideration. Also, a random disorder is chosen such that $T < 0.25$ to ensure that the multiple scattering is in the diffusion regime of wave transport.

continuity equation derived from the Helmholtz wave equation (where the total energy is conserved) is given as the following

Continuity equation based on the wave equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J}(r, t) = 0, \quad (3.11)$$

where the energy volume density, $\rho(r, t) = \frac{1}{2} \left[\frac{1}{c^2} \left(\frac{\partial E(r, t)}{\partial t} \right)^2 + |\nabla E(r, t)|^2 \right]$

and the energy current density, $\vec{J}(r, t) = \left[-\frac{\partial E(r, t)}{\partial t} \nabla E(r, t) \right]$

In 2D, $\vec{J}(r, t) = J_z(r, t)\hat{e}_z + J_y(r, t)\hat{e}_y$

Using the expression of current density $\vec{J}(r, t)$ obtained from the continuity equation, the total transmission (T) and reflection (R), propagating normal to the boundary surfaces shown in the Figure 3.5 can be evaluated as the following

Total transmission and reflection

$$T = \frac{\frac{1}{t_{cycle}} \int_{t=t_0}^{t=t_0+t_{cycle}} \int_{y=0}^{y=W} J_z^{trans}(z, y, t)|_{(z,y) \in \Gamma_R} dy dt}{\frac{1}{t_{cycle}} \int_{t=t_0}^{t=t_0+t_{cycle}} \int_{y=0}^{y=W} J_z^{source}(z, y, t)|_{(z,y) \in \Gamma_R} dy dt}$$

$$R = \frac{\frac{-1}{t_{cycle}} \int_{t=t_0}^{t=t_0+t_{cycle}} \int_{y=0}^{y=W} J_z^{refl}(z, y, t)|_{(z,y) \in \Gamma_L} dy dt}{\frac{1}{t_{cycle}} \int_{t=t_0}^{t=t_0+t_{cycle}} \int_{y=0}^{y=W} J_z^{source}(z, y, t)|_{(z,y) \in \Gamma_L} dy dt} \quad (3.12)$$

where $t_{cycle} = 2\pi/\omega_0$ is the time period of the wave, $J_z^{trans}(z, y, t)$ is the z component of the wave current density associated with the transmitted wave in presence of scatterers, $J_z^{refl}(z, t)$ is the z component of the wave current density associated with the reflected wave in presence of scatterers and $J_z^{source}(r, t)$ is z component of the wave current associated with the source wave, when no scattering perturbation against a background reference medium is present in the computational domain. Estimation of the source wave and the source current $J_z^{source}(r, t)$ at the boundaries (without the disorder), is done as a separate parallel run along with the FDTD time stepping for estimating the wave propagation in presence of the disorder. Sources in the FDTD method are formulated as soft dipole sources with a 180° phase difference between the excitations of the poles.¹⁴ Next, the estimation method¹⁵ for determining the amplitude and phase of the outgoing wave is discussed.

3.2.3 Estimation of the amplitude and phase of scattered wave for a stationary random medium

The phase conjugation of light pulses through random media has been modelled before[86] using the pseudo-spectral time domain method. For the phase conjugation using continuous wave sources, the steady-state amplitude and phase of the outgoing waves are estimated for a memory

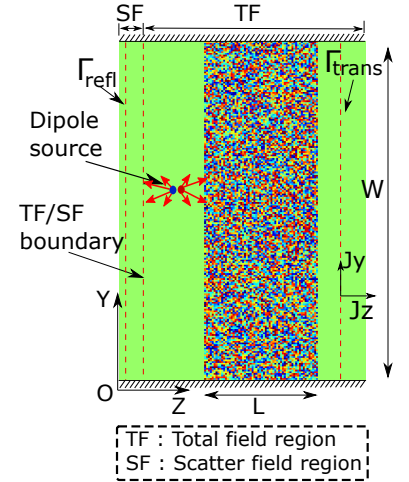


Figure 3.5: Geometry of the wave FDTD formulation is shown for the forward propagation.. The wave sources are implemented either as a single dipole or a phased array of dipoles. The transmission boundary Γ_{trans} is at the right side of the slab, reflection boundary Γ_{refl} at the left side of the slab and the total-field/scatter-field (TF/SF) boundary is placed on the left side of the source. The source wave (without the disorder) is subtracted in the SF region. Hence, only the reflected field from the slab completely passes through the TF/SF boundary into the SF region and gets detected at the Γ_{refl} surface as reflection. The current density $J(r, t)$ resolved along z and y are also shown.

14: For the dipole excitation involving point like sources, if the first point source of the dipole is excited as $E_0 \cos(\omega t)$, then the second point source, placed immediately to the right side, has to be of the form $E_0 \cos(\omega t + \pi)$ where E_0 is the amplitude.

15: In the FDTD method with continuous sources, the $E(r, t)$ data estimated at the transmission/reflection detection boundaries, is a spatially resolved time series data involving real E field values. For wavefront shaping application, the amplitude and phase of these harmonic waves resolved spatially have to be determined. Section 3.2.3 discusses the estimation method.

efficient¹⁶ modelling, instead of storing the outgoing field as a time series. This can be implemented by the phase sensitive detection (PSD) scheme given in [87] implemented in the context of seismic wave modelling.

Let $E_{trans}(z, y, t)|_{\Gamma_R} = E_0^{trans}(z, y)\cos(\omega_0 t + \phi_{trans}(z, y))$ be the outgoing time domain wave evaluated at the transmitting boundary Γ_R as shown in the Figure 3.5. Then, the amplitude and phase of the transmitted wave due to a single frequency continuous source can be estimated as the following. Let there be two temporal reference signals defined and known beforehand such that,

$$\begin{aligned} E_{0^\circ}^{ref}(t) &= E_{ref}\cos(\omega_0 t + \theta_{ref}) \\ E_{90^\circ}^{ref}(t) &= E_{ref}\cos(\omega_0 t + \theta_{ref} + \pi/2) \end{aligned} \quad (3.13)$$

$E_{0^\circ}^{ref}(t)$ is the in-phase reference signal and $E_{90^\circ}^{ref}(t)$ is the quadrature phase reference signal (which is 90° out of phase with the in-phase signal) with temporal frequency ω_0 . In the computational implementation, the amplitude E_{ref} can be set to unity and the phase θ_{ref} to be zero, for convenience. Next step is to measure the spatially resolved temporal cross-correlation of the transmitted wave $E_{trans}(r, t)|_{\Gamma_R}$ with that of the in-phase reference signal and the quadrature phase reference signal, over a time cycle[87].

$$\begin{aligned} X_{corr}(z, y)|_{(z,y) \in \Gamma_R} &= \frac{1}{t_{cycle}} \int_{t=t_0}^{t=t_0+t_{cycle}} E_{0^\circ}^{ref}(t) E_{trans}(z, y, t)|_{(z,y) \in \Gamma_R} dt \\ Y_{corr}(z, y)|_{(z,y) \in \Gamma_R} &= \frac{1}{t_{cycle}} \int_{t=t_0}^{t=t_0+t_{cycle}} E_{90^\circ}^{ref}(t) E_{trans}(z, y, t)|_{(z,y) \in \Gamma_R} dt \end{aligned} \quad (3.14)$$

where $t_{cycle} = 2\pi/\omega_0$ is the time period of the wave. Then, the amplitude $E_0^{trans}(z, y)|_{(z,y) \in \Gamma_R}$ and the phase $\phi_{trans}(z, y)|_{(z,y) \in \Gamma_R}$ of the transmitted wave $E_{trans}(z, y, t)|_{(z,y) \in \Gamma_R}$ can be reconstructed as the following

Phase sensitive detection

$$\begin{aligned} E_0^{trans}(z, y)|_{(z,y) \in \Gamma_R} &= 2\sqrt{X_{corr}(z, y)^2 + Y_{corr}(z, y)^2}/E_{ref} \\ \phi_{trans}(z, y)|_{(z,y) \in \Gamma_R} &= \tan^{-1}(Y_{corr}(z, y)/X_{corr}(z, y)) + \theta_{ref} \end{aligned} \quad (3.15)$$

In *Matlab*, the $\text{atan2}(Y, X)$, the four-quadrant inverse tangent function could be used to estimate $\phi_{trans}(z, y)|_{(z,y) \in \Gamma_R}$. Thus, the amplitude and phase of transmitted wave are estimated. Similarly, the amplitude and phase for the reflected wave and the source wave (without any dielectric perturbation) is estimated. For the forward propagation of wave transport shown in Figure 3.8(a), the phase sensitive detection technique applied to estimate the transmitted, reflected and the source wave amplitude and phase, yields the results shown in Figure 3.6(a), Figure 3.6(b) and Figure 3.6(c), respectively. Such an estimation of the transmitted wave amplitude and phase, is to implement the phase conjugation operation to focus back at the source location. The phase conjugate source is injected at the same plane as an array of dipoles, where the transmission in the forward propagation was estimated. The details on focussing through

16: Using the phase sensitive lock-in detection scheme to determine the amplitude and phase of the outgoing wave, requires only a single cycle of the outgoing wave upon achieving steady state during the wave propagation. Hence, the outgoing waves need not be stored for large time durations for the eventual purpose of time reversing the waves to obtain a focus.

[87]: Nihei et al. (2007), 'Frequency response modelling of seismic waves using finite difference time domain with phase sensitive detection (TD-PSD)'

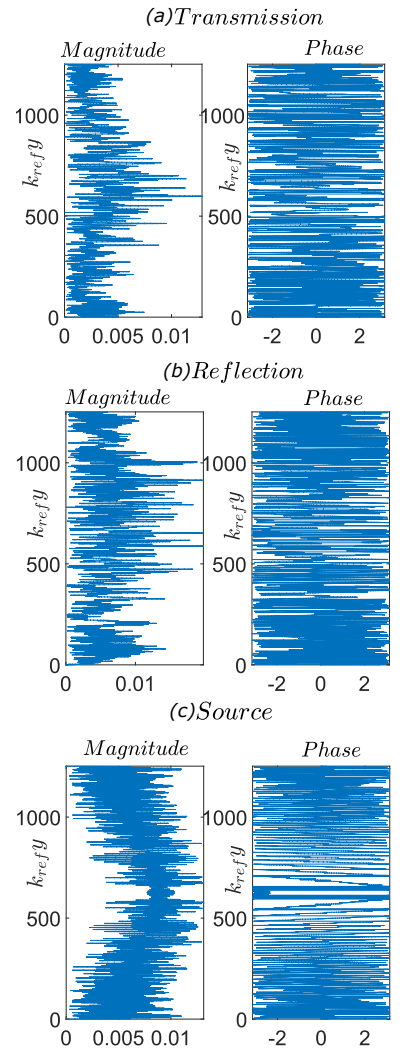


Figure 3.6: The spatially resolved amplitude and wrapped phase of the (a) transmitted wave estimated using the equation 3.15 associated with the Phase sensitive detection (PSD) scheme, for the wave transport scenario shown in Figure 3.8(a) and the sample given in Figure 3.7, is plotted. Similarly, PSD estimation for (b) the reflected wave and (c) the source wave on the transmitted side are also given.

phase conjugation is explained in the following section.

3.3 Wavefront shaping : Focussing through phase conjugation

This section demonstrates the wavefront shaping applications of focussing through a stationary disorder given in Figure 3.7. The single speckle focussing is explained as the following, which involves phase conjugation onto the source location from which the wave was originated.

3.3.1 Single speckle focussing

Time reversed focussing onto a small focal region (typically of the order the size of a wave speckle) through a diffusive disorder, has been reported in different physical domains. The earliest attempt[88] of the practical realisation of the concept of time-reversal was using transient acoustic waves involving an acoustic time-reversal mirror. For a detailed review on time-reversed acoustics, refer to[89]. The application involving electromagnetic waves[90] followed, where a quasi monochromatic electromagnetic pulse in the *GHz* range was time reversed to focus in a reverberant room. Focussing of coherent light through a disordered medium was first reported by Vellekoop and Mosk[1] using spatial light modulators (*SLM*), by feedback-optimisation of the phase of the monochromatic incident light to overcome strong multiple scattering. Deriving ideas from several phase conjugation experiments¹⁷, modelling aspects of focussing using time-reversal (or phase conjugation for a monochromatic wave) is discussed in this section. Once the amplitude and phase of the transmitted wave is determined as per the phase sensitive detection method explained in Section 3.2.3, the transmitted wave can be time reversed by setting $t = -t$ and time stepping the transmitted wave $E_{trans}(r, -t)|_{\Gamma_R}$ as the phase conjugate wave, injected at the transmission boundary Γ_R (as a one way source), as shown in the Figure 3.8(b). Three main properties are observed.

1. The disorder helps in attaining high spatial resolution while focussing on phase conjugation. The focal spot has a size of the order $\lambda/2$, as shown in the Figure 3.8(b) and Figure 3.9(c), which is typically the size of a speckle spot[93, 94]. Hence, a random disorder incident upon by a phase conjugate wave, operates equivalent to a larger-aperture scattering-lens, approaching the diffraction limit for focussing.
2. Total transmission value is $\approx 2/3$ upon phase conjugation, which a universal constant[95], when the transmitted wave during forward propagation is completely measured without any loss in the detection. Such a universal value is independent of the non absorbing sample thickness/microscopic scattering properties in the diffusion regime (under the condition that total transmission $T < 0.25$).
3. The Focussing contrast $C_f = \frac{\text{peak intensity}}{\text{average background intensity}}$ is of the order of -20 dB as shown in the Figure 3.9 which is the field profile obtained from Figure 3.8(b).

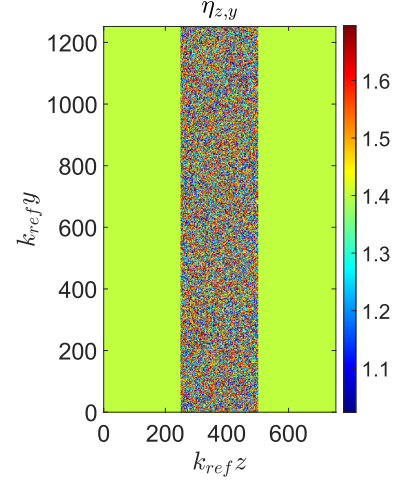


Figure 3.7: Disorder refractive index distribution (uniform distribution) $\eta_{z,y}$ used for FDTD wave propagation is shown. $k_{ref}L = 251.0163$, $k_{ref}W = 1251.8$, reference medium refractive index of $\eta_{ref} = 1.4$, source frequency $f_{src} = 3.2 \times 10^{14}$, wavelength in the reference region $\lambda_{ref} = 669.18$ nm, $\max[\eta(z, y)] = 1.6947$, $\min[\eta(z, y)] = 1.0237$ and $k_{ref}\Delta_z = k_{ref}\Delta_y = 0.2076$.

17: The experimental phase conjugation of light can be performed using different methods. [91] used a photorefractive $LiNbO_3$ crystal to perform a holographic recording of the transmitted field through a scattering medium and perform phase conjugation through the same scatterer by playing the phase conjugate wave back using a reference beam. [92] used the digital optical phase conjugation (DOPC) scheme where a spatial light modulator (SLM) was used to playback the phase conjugate wave through the scattering medium. [8] measured the optical transmission matrix of a scattering medium and estimated the phase conjugate wave for focussing, using the information contained in the measured transmission matrix.

[91]: Yaqoob et al. (2008), ‘Optical phase conjugation for turbidity suppression in biological samples’

[92]: Cui et al. (2010), ‘Implementation of a digital optical phase conjugation system and its application to study the robustness of turbidity suppression by phase conjugation’

[8]: Popoff et al. (2010), ‘Measuring the transmission matrix in optics: an approach to the study and control of light propagation in disordered media’

[95]: Vellekoop et al. (2008), ‘Universal optimal transmission of light through disordered materials’

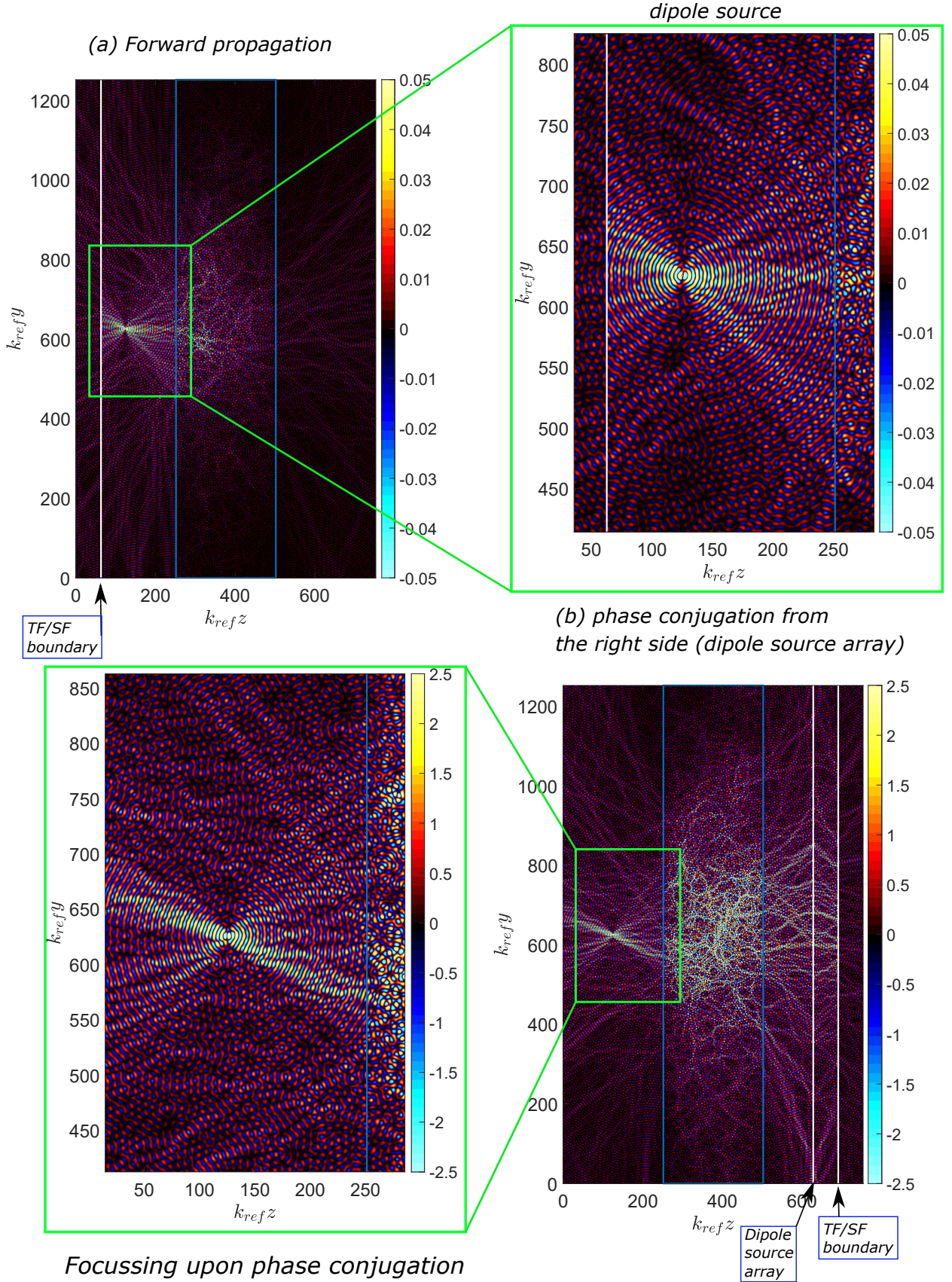


Figure 3.8: Forward propagation and phase conjugation of a wave in a disordered medium (in the diffusion regime) are shown. (a) The forward propagation of the wave due to a dipole source placed together with a total-field/scatter-field (TF/SF) boundary at the left side of the disorder is shown. For the forward propagation, the total transmission, $T = 0.2410$, reflection, $R = 0.7544$ and $T + R = 0.9954$. The corresponding disorder is shown in Figure 3.7. The phase sensitive detection (given in Section 3.2.3) of the amplitude and phase of the transmitted, reflected and the source wave, are shown in Figure 3.6(a), (b) and (c), respectively. **(b)** Single speckle focussing (described in Section 3.3.1) through phase conjugation from right side of the disorder is shown. The total transmission upon phase conjugation, $T = 0.6729$ (approximately around the ensemble averaged transmission value of $2/3$), reflection, $R = 0.3310$ and $T + R = 1.0040$. The field plots associated with both the forward propagation and the phase conjugation have clipped colour map limits as shown, to make the transport paths visible. For the actual order of the intensity around the focus and the background, refer to Figure 3.9.

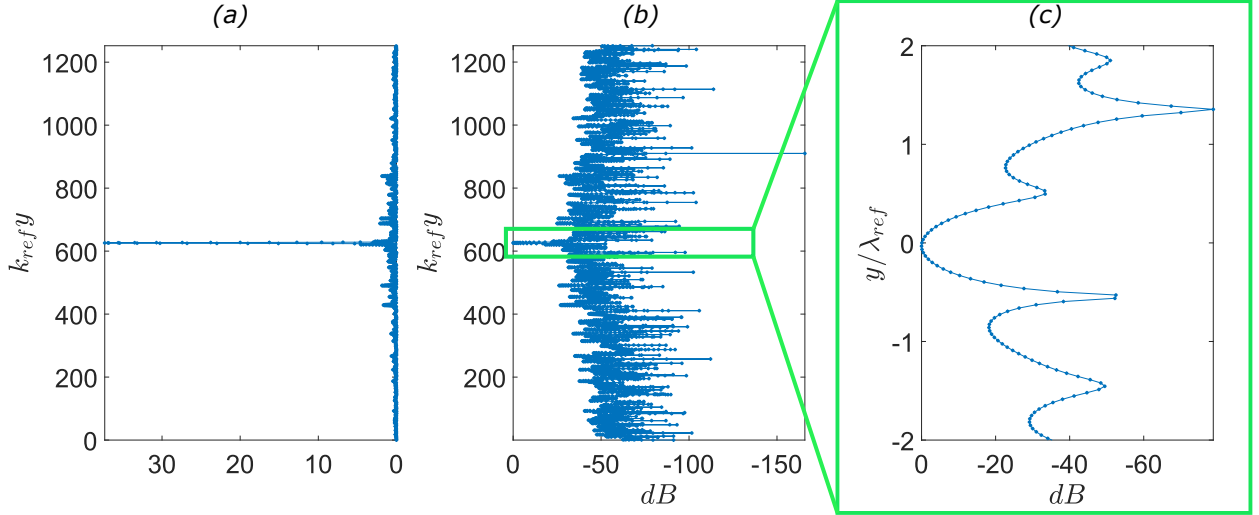


Figure 3.9: Transmitted field intensity profile at the focus during phase conjugation is plotted. (a) The field intensity at the plane of focus during the phase conjugation operation as shown in the Figure 3.7(b). (b) The decibel plot of the field intensity, normalised with respect to the peak intensity is shown. The background around and below -20 dB level is seen. (c) Figure 3.9(b) zoomed around the focus to show the -6 dB full-width half maximum width approximately of the order of $\approx \lambda_{ref}/2$, where $\approx \lambda_{ref} = \lambda_0/\eta_{ref}$ and λ_0 the free-space wavelength.

For both the forward propagation and the phase conjugation shown in Figure 3.8 (a) and (b), the sources are implemented as dipole sources instead of monopoles. This is mainly to direct the point source along the longitudinal direction (z direction) and minimise¹⁸ transverse oscillation of the source wave along y direction. For the results shown in Figure 3.8 (a) and (b), a stationary disorder was used. But in case of biological tissue, there could be random particle motion inside the medium, which affects the stability of the focus for a given phase conjugate wave estimated from the forward propagation. Hence, in the next section, de-focussing of a given phase conjugate wave due to random Brownian motion is studied in terms of various dimensionless scalable parameters.

3.4 Effect of sample decorrelation on the stability of the focus

In this section, the role played by the sample decorrelation due to Brownian motion on the stability of focus^[80] attained by wavefront shaping in dynamical media is studied. As shown in Figure 3.2, the analysis is divided into two main parts involving two kinds of *FDTD* formulations. The first kind is the *FDTD* time-stepping which is done on the Langevin equation to induce the Brownian motion on the scattering particles, creating an ensemble of particle spatial configuration states. The second *FDTD* routine is for time stepping the wave transport phenomena as explained in the previous sections. The random Brownian force acting on the particles¹⁹ is parametrised by the particle diffusion constant D_B , through the well-known fluctuation-dissipation theorem.²⁰ If the random force acting on a particle is known along with the frictional drag coefficient, then the temporal evolution of the particle position can be estimated. The mean square displacement averaged over many particles (as an implicit function of time) $MSD(t) = \langle |\vec{r}(t) - \vec{r}(0)|^2 \rangle$ can be calculated where $\vec{r}(t)$ is the position vector as a function of time. For

18: This is because the transverse boundaries are reflecting boundaries and any prolonged oscillation of waves along transverse direction (especially generated, if monopole sources are implemented) causes *FDTD* flux conservation ($R + T = 1$) to converge at a slower rate with respect to the total number of time-stepping needed for attaining steady-state.

[80]: Blochet et al. (2019), ‘Enhanced stability of the focus obtained by wavefront optimization in dynamical scattering media’

19: Particles are mono-disperse with a given radius and the refractive index is taken to be uniform across all the particles.

20: The fluctuation-dissipation theorem is a topic discussed under the context of non-equilibrium statistical mechanics. For proof and discussion, one may refer to equation 1.12 of chapter 1, [96] or equation 3.14 of chapter 3, [97].

[96]: Zwanzig (2001), *Nonequilibrium statistical mechanics*

[97]: Balakrishnan (2008), *Elements of nonequilibrium statistical mechanics*

representational convenience, the dimensionless $MSD(t)$ is defined as $MSD(t) = \langle k_{ref}^2 |\vec{r}(t) - \vec{r}(0)|^2 \rangle$ and this form will be used throughout this chapter. The particles in this chapter are modelled as soft particles (without hard collisions) instead of the hard collidable version, mainly for the simplicity of the numerical implementation. The Brownian spatial trajectory for all the soft particles undergoing Brownian motion, according to the Langevin equation, is stored for each time-steps, thus forming an ensemble of particle spatial configuration states (numbered 0, 1, 2, 3 etc.). A focus can be created by the phase conjugation onto a point source using the first particle spatial configuration state (numbered 0). The temporal stability of the focus with respect to sample Brownian motion can be estimated by performing separate *FDTD* wave transport modelling for each of the remaining particle spatial configuration states (numbered 1, 2, 3, 4 etc.), one after the other. The following section explains the *FDTD* formulation for the Langevin equation for time-stepping the Brownian particle motion.

3.4.1 *FDTD* formulation of the Langevin equation for Brownian motion

Let the position vector $\vec{r}$ as a function of time t is given as $\vec{r}(t) = z(t)\hat{e}_z + y(t)\hat{e}_y$. The 2D Langevin equation for a single scattering particle can then be written for each of the Cartesian position components as the following

2D Langevin equation for the single particle Brownian motion

$$m \frac{d^2}{dt^2} \begin{bmatrix} z(t)\hat{e}_z \\ y(t)\hat{e}_y \end{bmatrix} = -\gamma \frac{d}{dt} \begin{bmatrix} z(t)\hat{e}_z \\ y(t)\hat{e}_y \end{bmatrix} + \begin{bmatrix} f_r^z(t)\hat{e}_z \\ f_r^y(t)\hat{e}_y \end{bmatrix} \quad (3.16)$$

where m is the mass of the particle, $\hat{e}_z$ and $\hat{e}_y$ the unit vectors along z and y , γ is the friction coefficient associated with the Brownian motion, f_r^z is the z component and f_r^y is the y component of the random Brownian force acting on the particle. Although the force components f_r^y and f_r^z fluctuate randomly in time, its statistical property such as the temporal autocorrelation function is a known deterministic function as given below

$$\langle f_r^z(t) f_r^z(t') \rangle = \langle f_r^y(t) f_r^y(t') \rangle = 2B\delta(t - t') \quad (3.17)$$

where $B = KT\gamma$ from the fluctuation-dissipation theorem such that K is the Boltzmann constant and T the temperature. Equation 3.17 implies that the random force components are delta correlated in time. The Brownian diffusion constant $D_B = (KT/\gamma)$ can be set to control the B parameter appearing in the autocorrelation function and eventually leading it to the definition of the random force components f_r^y and f_r^z used in the numerical implementation. The section 2.2 of [98] describes a method by which the random force component f_r^y or f_r^z , obeying the Brownian autocorrelation function given in 3.17, could be numerically generated. First, a uniformly distributed and uncorrelated random number *rand*, spread in the interval $[-0.5, 0.5]$ is defined to generate a delta-correlated

[98]: Grassia et al. (1995), 'Computer simulations of Brownian motion of complex systems'

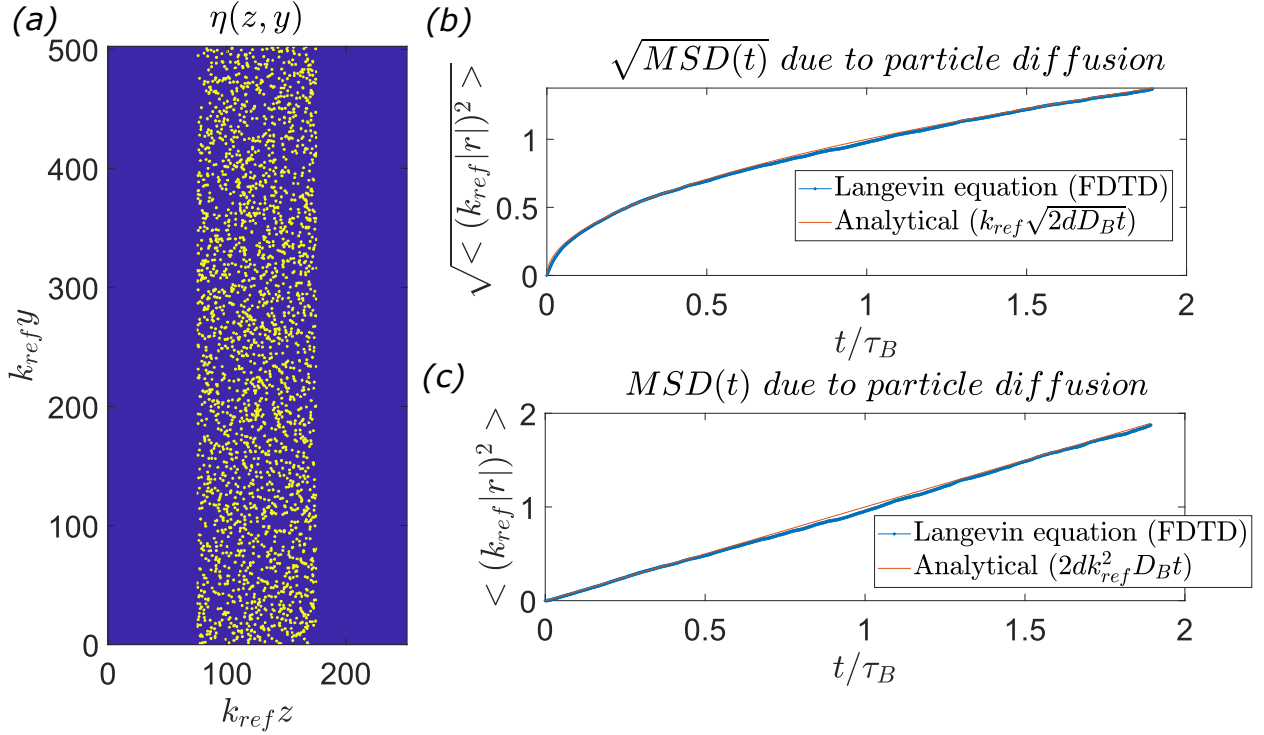


Figure 3.10: The Langevin FDTD formalism for the Brownian particle motion is demonstrated. (a) Geometry of the scattering problem involving Brownian particles is shown. Monodisperse Brownian particles (2500 in number) have a common dimensionless diameter of $2k_{ref}r_B = 2.011$ and same refractive index of 2.2782, against a background refractive index of 1.3. Every particle shown undergoes Brownian motion as per the Langevin FDTD equations 3.20 and 3.21. (b) The square root of the dimensionless Mean Squared Displacement (MSD) as a function of the dimensionless time t/τ_B where τ_B is the Brownian time constant is plotted. The Brownian time constant τ_B is defined (chapter 9 of [17]) as $\tau_B = 1/(4D_Bk_{ref}^2)$. The plotted curve is the average dimensionless MSD, averaged over all the Brownian particles. D_B is the Brownian diffusion constant (m^2/s), $k_{ref}^2D_B$ has the dimension of $(1/s)$ and $d = 2$ is the dimensionality of the problem being 2D. (c) Similarly, the plot for the dimensionless $MSD(t)$ is also shown, which has a linear behaviour with respect to t/t_B .

time-series for the force components f_r^y and f_r^z . Due to a known property of the autocorrelation function that its maximum value at the zero lag ($t - t' = 0$) is the variance of the time series, the f_r^y or f_r^z time series generated using the *rand* function, has to have the right variance corresponding to the equation 3.17. Hence, first normalise the *rand* random variable²¹ to have unit variance by dividing it with the standard deviation $1/\sqrt{12}$ of a uniformly distributed random variable in $[-0.5, 0.5]$. Secondly, from equation 3.17, variance of the time series has to be $2B/dt = 2KT\gamma/dt$, which²² is the maximum value of the auto-correlation function at the zero lag ($t - t' = 0$). Hence, the standard deviation $\sqrt{2B/dt} = \sqrt{2KT\gamma/dt}$ should be multiplied onto the normalised *rand*/($1/\sqrt{12}$) value, yielding the following definition for the random force components as a random variable[98]

$$\begin{aligned} f_r^z = f_r^y &= \sqrt{\frac{2KT\gamma}{dt}} \left\{ \frac{rand}{\frac{1}{\sqrt{12}}} \right\} \\ &= \left\{ \sqrt{\frac{24KT\gamma}{dt}} \right\} rand \end{aligned} \quad (3.18)$$

Then, the finite difference formulation of the Langevin equation can be obtained as the following. First, solve for the z position Cartesian component and the analysis for the y position Cartesian component

21: *rand* random variable has zero mean and is uniformly distributed between $[-0.5, 0.5]$ with a variance of $1/12$.

22: $1/dt$ came from the discrete version of the Dirac-delta function given in equation 3.17.

follows the same as that of the z component. Applying the central difference scheme on the first and the second order temporal derivative of the z position component given in equation 3.17,

$$\begin{aligned} m \frac{d^2}{dt^2} z(t) &= -\gamma \frac{d}{dt} z(t) + f_r^z(t) \Rightarrow \\ m \left(\frac{z^{n+1} - 2z^n + z^{n-1}}{\Delta_t^2} \right) &= -\gamma \left(\frac{z^{n+1} - z^{n-1}}{2\Delta_t} \right) + f_r^{z,n} \end{aligned} \quad (3.19)$$

where n is the time step index and $f_r^{z,n}$ is the n^{th} random variable drawn from the equation 3.18. Solving for z^{n+1}

FDTD time stepping equation for the single particle Langevin equation in 2D

$$z^{n+1} = \left(\frac{4m}{2m + \gamma\Delta_t} \right) z^n + \left(\frac{-2m + \gamma\Delta_t}{2m + \gamma\Delta_t} \right) z^{n-1} + \left(\frac{2\Delta_t^2}{2m + \gamma\Delta_t} \right) f_r^{z,n} \quad (3.20)$$

Similarly, for the y position Cartesian component,

$$y^{n+1} = \left(\frac{4m}{2m + \gamma\Delta_t} \right) y^n + \left(\frac{-2m + \gamma\Delta_t}{2m + \gamma\Delta_t} \right) y^{n-1} + \left(\frac{2\Delta_t^2}{2m + \gamma\Delta_t} \right) f_r^{y,n} \quad (3.21)$$

23: Soft Brownian particles (taken as an assumption in the modelling) imply that the particles pass over each other without any hard collision interactions. Such an assumption is taken for the simplicity and easiness of modelling, as the implementation of the hard collision of Brownian particles may be an unnecessary sophistication for the intended goals of this section. Also, the particles don't flow out of the grid boundaries. Upon crossing the boundary, the numerical implementation ensures that the particles rebounds to the interior.

Although the equations given in 3.20 and 3.21 are given for a single particle, the same equations could be applied on a collection of "soft"²³ particles independently. Here the term "soft" refers to the assumption that the particles don't interact with each other and pass over one another without any hard collision. The particle starting position (z_0, y_0) is initialised randomly for all the particles within the computational domain and time stepping equations 3.20 and 3.21 are used to obtain their individual trajectories, beginning from the starting position. The results associated with such a FDTD time-stepping, on all the Brownian particles, are given in Figure 3.10. As indicated in the Figure 3.10(c), due to the linear relationship between dimensionless time t/τ_B and $MSD(t)$, either the term t/τ_B or the term $MSD(t)$ can be interchangeably used to study the dependence of wave focussing through wavefront shaping and the parameters involved with that of the Brownian motion. Here, the Brownian time constant τ_B is defined as $\tau_B = 1/(4D_B k_{ref}^2)$ following the definition given in chapter 9 of [17]. Next section studies such a role played by Brownian motion, on the stability of the single speckle focussing attained by phase conjugation.

3.4.2 Single speckle focussing vs Brownian motion

First, just using the first particle configuration state of the Brownian particles, a focus is generated by phase conjugation as shown in the Figure 3.11(a), using the methodology given in Section 3.3.1. For creating such a focus, the disorder is taken to be stationary without any Brownian

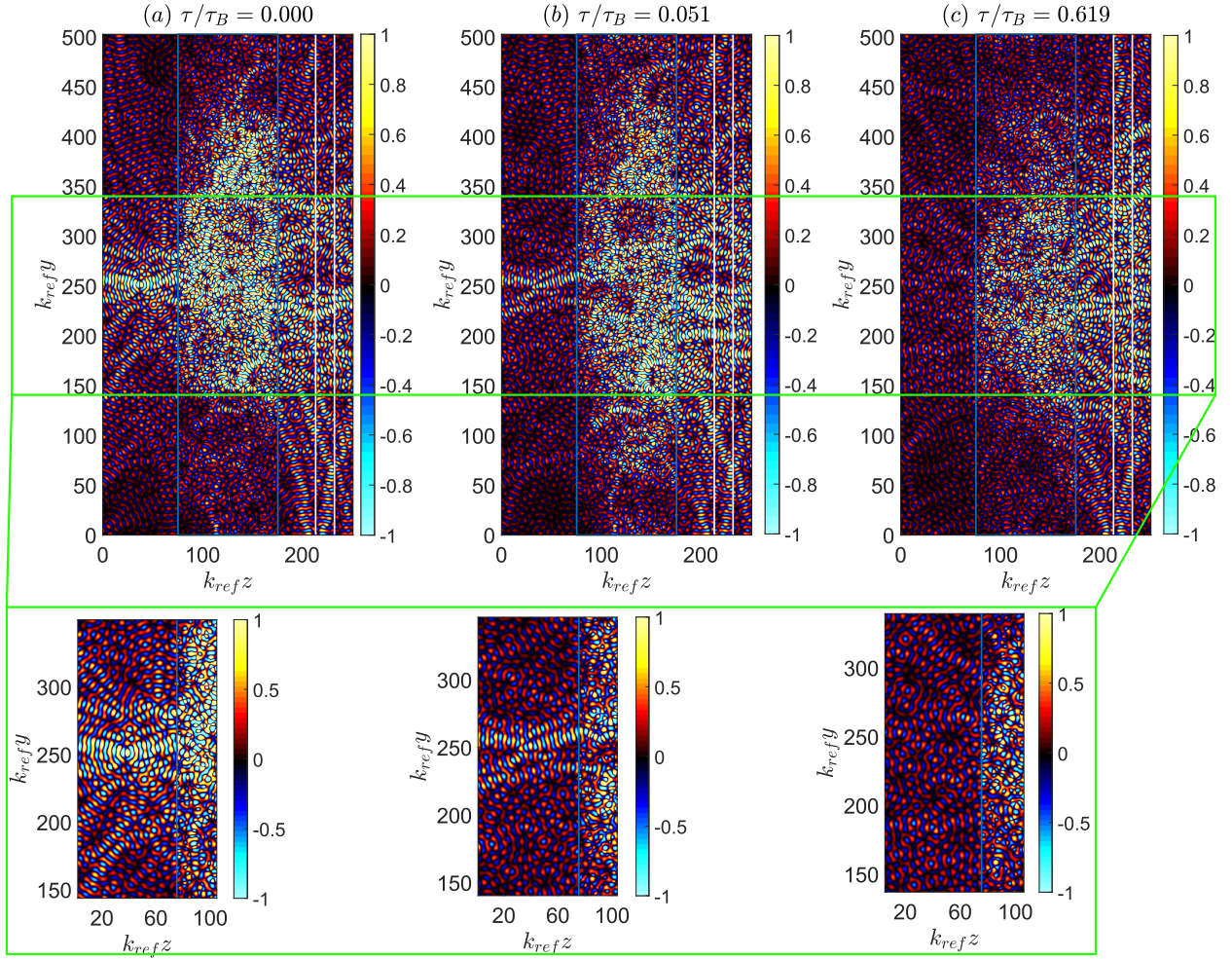


Figure 3.11: The single speckle focussing and the decorrelation effect of the obtained focus, due to the Brownian motion are plotted. Three instances of focussing are shown, starting with a disorder in the diffusion regime (with an unshaped transmission of $T = 0.2269$, reflection, $R = 0.7829$ and $T + R = 1.0098$). (a) At $\tau/\tau_B = 0$, a wave focus is attained via phase conjugation with a transmission of $T = 0.6769 \approx 2/3$, $R = 0.3247$ and $T + R = 1.0016$, where $\tau_B = 1/(4D_B k_{ref}^2)$ is the Brownian time constant as discussed before. But, in the onset of Brownian motion, the single speckle focus starts to get defocussed as expected, as shown in (b) where $\tau/\tau_B = 0.051$, $T = 0.3385$, $R = 0.6654$, $T + R = 1.0039$ and (c) finally, for $\tau/\tau_B = 0.619$, the focal spot gets defocussed fully where $T = 0.2370$, $R = 0.7689$, $T + R = 1.0059$. All these field plots have clipped colour map limits as shown to make the transport paths visible. For the plots involving the total transmission and the peak intensity, against the Brownian evolution of the disorder, refer Figure 3.12.

motion incorporated. Once such a focus is created, different runs of wave *FDTD* simulations are done separately by changing the particle configuration states obtained by the Langevin *FDTD* time-stepping of the Brownian motion, using the same phase conjugate wave used for creating the focus which involved the first (initial) particle configuration state. Such a formulation of wave transport using different separate runs of particle configuration state in which the wave attains steady state for each of the runs individually, can be referred to as a quasi-static approximation. Each particle configuration state has its own t/τ_B or a dimensionless $MSD(t)$ associated, with respect to the initial or the first particle spatial configuration state. As shown in Figure 3.11 b) and c), as time progresses, the Brownian motion scrambles the incident wavefront which was originally used for focussing and eventually the sharp focus disappears. For the quantitative measures involving such a defocussing due to disorder decorrelation, refer to Figure 3.12.

For a disordered sample with an unshaped transmission of the order of

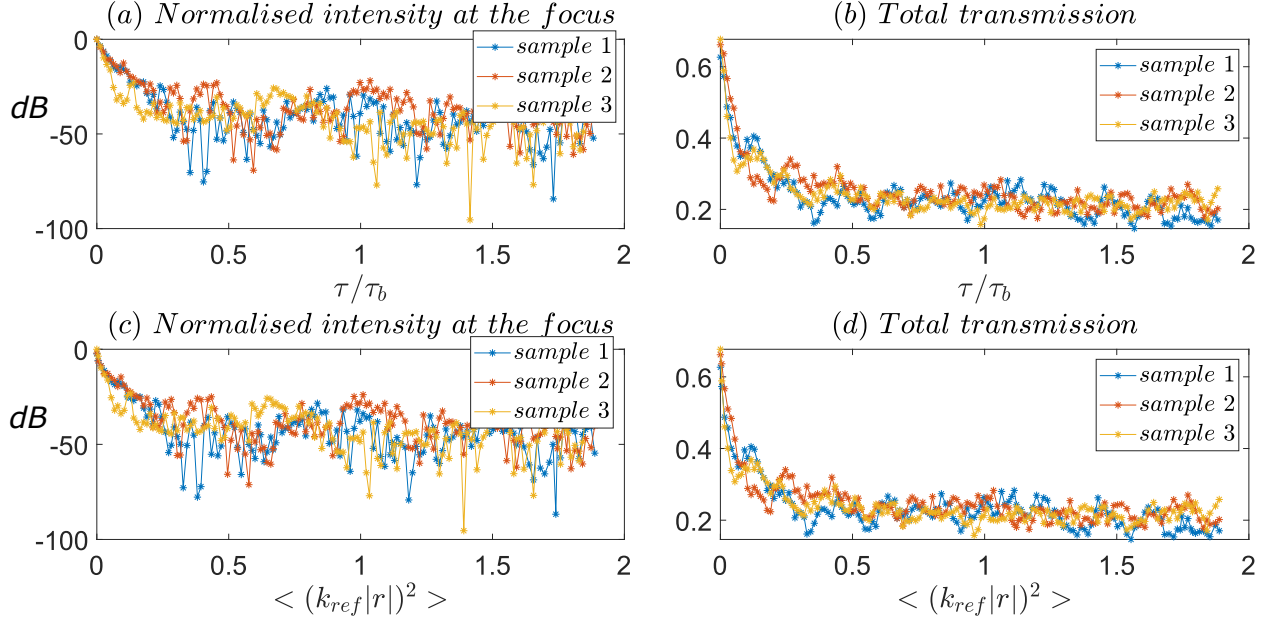


Figure 3.12: Evolution of the normalised peak intensity and the total total transmission during phase conjugation for focussing, due to the Brownian motion (as shown in Figure 3.11), are plotted. Reduction of the peak intensity at the focus is shown against the (a) dimensionless time, t/τ_B and (c) the dimensionless $MSD(t)$. Similarly, the reduction of the phase conjugated total transmission, due to the Brownian motion is plotted in (b) and (d). Three samples having similar unshaped transmission of 0.2349, 0.2017 and 0.2269, are used. Transmission upon phase conjugation, just before the initiation of the Brownian motion are 0.6268, 0.6616, and 0.6769 for sample 1, 2 and 3, respectively.

0.2349, the total transmission drops from $\approx 2/3$ to the average unshaped transmission value, within t/τ_B or $\langle (k_{ref}|r|)^2 \rangle$ value of 0.5 as shown in the Figure 3.12 (b) and (c). Similarly, the peak intensity formed due to the focus also fades away and gets disappeared within the averaged background as shown in the Figure 3.12(a) and (c). This quantifies the stability or the sensitivity of the focus for diffusive transmission in the regime around a transmission value of 0.22, against the Brownian motion. This also point out the experimental challenge to perform single speckle focussing in media with fast Brownian dynamics in the light transmission diffusion regime.

Until now, wave focussing outside a disordered region was discussed. Next section deals with a relevant time dependent phenomena in the context of wavefront shaping referred to as the space-time modulation (STM), which is a generalisation to the acousto-optic effect, to be used as a “guide-star” to focus light inside the disorder.

3.5 Finite difference Time domain (FDTD) formulation of the wave equation for a Space-Time Modulated (STM) medium

Single speckle focussing via phase conjugation through a random medium was presented before. In such a method of focussing, the focal spot formed due to the phase conjugated wave was outside the random media. In some cases, it is desirable to have the focussed region to lie within the random medium. Such a geometry will be particularly

suitable for tomography applications in random media, by creating a focussed source inside. This is experimentally achieved by incorporating a “guide-star”[26] inside the random medium, which serves as the reference region where we desire to focus through. The guide-star could be based on focussed ultrasound[27], fluorescence [99] or nano-particles[100]. In the following section, the finite difference scheme for implementing the effects of acousto-optic modulation as a guide-star is explained. An *FDTD* scheme was reported by[28] for modelling an acousto-optic region as a guide-star. In this chapter, a different perspective of looking at the same problem is presented, which involves a space time modulated (*STM*) region operating in the Raman-Nath regime and the phase sensitive detection of the modulated harmonic wavefronts.

The generalised theoretical framework used for modelling the effects of acousto-optic modulation is referred to as wave propagation in the space-time modulated medium. Refer [82, 101] for a detailed review regarding the theory and applications of space-time modulated systems. When a carrier wave at temporal frequency ω_0 interacts with a *STM* region represented by $\epsilon_r(r, t)$, temporally harmonic wavefronts emerges due to the interaction. In this chapter, $\epsilon_r(r, t)$ is configured to have only one temporal frequency, ω_{mod} . Then, the harmonic wavefront components (otherwise referred as side-band wavefronts) emerging from the *STM* region have temporal frequencies $(\dots\omega_0 - 3\omega_{mod}, \omega_0 - 2\omega_{mod}, \omega_0 - \omega_{mod}, \omega_0 + \omega_{mod}, \omega_0 + 2\omega_{mod}, \omega_0 + 3\omega_{mod}, \dots)$. Next, the *FDTD* formulation of the generalised wave equation (equation 3.1) with time dependent dielectric constant $\epsilon_r(r, t)$ is presented.

Generalised Time-domain Helmholtz wave equation

$$\nabla^2 E(r, t) - \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} (\epsilon_r(r, t) E(r, t)) = 0 \quad (3.22)$$

Using the product rule for the second order temporal derivative, equation 3.22 can be expanded as

$$\begin{aligned} \nabla^2 E(r, t) &= \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} (\epsilon_r(r, t) E(r, t)) \\ &= \frac{1}{c_0^2} \left\{ \epsilon_r(r, t) \frac{\partial^2}{\partial t^2} E(r, t) + 2 \left(\frac{\partial}{\partial t} \epsilon_r(r, t) \right) \frac{\partial}{\partial t} E(r, t) + E(r, t) \frac{\partial^2}{\partial t^2} \epsilon_r(r, t) \right\} \end{aligned} \quad (3.23)$$

To obtain the discrete version of the above given equation (similar to that of section Section 3.2), following operator notations $D_n[\dots]$ and $D_n^2[\dots]$, representing the first order and the second order temporal derivatives, are presented in the side note²⁴ which could be used for simplification

[26]: Horstmeyer et al. (2015), ‘Guidestar-assisted wavefront-shaping methods for focusing light into biological tissue’

[27]: Xu et al. (2011), ‘Time-reversed ultrasonically encoded optical focusing into scattering media’

[99]: Si et al. (2012), ‘Fluorescence imaging beyond the ballistic regime by ultrasound-pulse-guided digital phase conjugation’

[100]: Hsieh et al. (2010), ‘Digital phase conjugation of second harmonic radiation emitted by nanoparticles in turbid media’

[82]: Taravati et al. (2019), ‘Generalized space-time-periodic diffraction gratings: Theory and applications’

[101]: Taravati et al. (2020), ‘Space-time modulation: Principles and applications’

24: Operator notations $D_n[\dots]$ and $D_n^2[\dots]$, representing the first order and second order temporal derivatives used to discretise equation 3.23, are given as the following

$$\epsilon_r(z, y, t)|_{t=(n-1)\Delta t} = \epsilon_{r,i,j}^n \quad (3.24)$$

$$\begin{aligned} \frac{\partial}{\partial t} \epsilon_r(z, y, t)|_{t=(n-1)\Delta t} &= \\ \left(\frac{\epsilon_{i,j}^{n+1} - \epsilon_{i,j}^{n-1}}{2\Delta t} \right) &= D_n \left[\epsilon_{r,i,j}^n \right] \end{aligned} \quad (3.25)$$

$$\begin{aligned} \frac{\partial^2}{\partial t^2} \epsilon_r(z, y, t)|_{t=(n-1)\Delta t} &= \\ \left(\frac{\epsilon_{i,j}^{n-1} - 2\epsilon_{i,j}^n + \epsilon_{i,j}^{n+1}}{\Delta t^2} \right) &= D_n^2 \left[\epsilon_{r,i,j}^n \right] \end{aligned} \quad (3.26)$$

purposes. Then, the discrete form of equation 3.23 can be written as,

$$\left\{ \frac{E_{i,j-1}^n + E_{i,j+1}^n - 2E_{i,j}^n}{\Delta_y^2} \right\} + \left\{ \frac{E_{i-1,j}^n + E_{i+1,j}^n - 2E_{i,j}^n}{\Delta_z^2} \right\} = \frac{1}{c_0^2} \left\{ \frac{(E_{i,j}^{n-1} + E_{i,j}^{n+1} - 2E_{i,j}^n) \epsilon_{r_{i,j}}^n}{\Delta_t^2} + \frac{2(E_{i,j}^{n+1} - E_{i,j}^{n-1}) D_n [\epsilon_{r_{i,j}}^n]}{2\Delta_t} + E_{i,j}^n D_n^2 [\epsilon_{r_{i,j}}^n] \right\} \quad (3.27)$$

Let $\Delta_z = \Delta_y = \Delta_s$ and rearranging the above equation to define parameters w_0 , w_1 and w_2

$$\underbrace{\left\{ \frac{E_{i-1,j}^n + E_{i+1,j}^n - 2E_{i,j}^n}{\Delta_s^2} \right\}}_{w_0} + \underbrace{\left\{ \frac{(E_{i,j}^{n-1} + E_{i,j}^{n+1} - 2E_{i,j}^n) \epsilon_{r_{i,j}}^n}{(c_0 \Delta_t)^2} \right\}}_{w_1} + \underbrace{\left\{ \frac{2(E_{i,j}^{n+1} - E_{i,j}^{n-1}) D_n [\epsilon_{r_{i,j}}^n]}{c_0^2 \Delta_t} + \frac{\Delta_s^2 D_n^2 [\epsilon_{r_{i,j}}^n]}{c_0^2} \right\}}_{w_2} E_{i,j}^n = \quad (3.28)$$

Using the defined terms w_0 , w_1 and w_2 , a time-stepping equation can be formed (similar to that of section Section 3.2) for $E_{i,j}^{n+1}$, in terms of $E_{i,j}^n$ and $E_{i,j}^{n-1}$, by rearranging²⁵ the equation 3.28.

25: If there is no time dependence for the dielectric constant $\epsilon_r(r, t)$, then the STM modulation gets nullified and $w_1 = w_2 = 0$ due to the reason that the temporal derivatives $D_n [\epsilon_{r_{i,j}}^n]$ and $D_n^2 [\epsilon_{r_{i,j}}^n]$ reduces to zero, recovering the equation 3.6 for a temporally stationary medium.

FDTD time stepping equation involving a STM region

$$E_{i,j}^{n+1} = \left(\frac{2w_0 - w_2}{w_0 + w_1} \right) E_{i,j}^n - \left(\frac{w_0 - w_1}{w_0 + w_1} \right) E_{i,j}^{n-1} + \left(\frac{1}{w_0 + w_1} \right) \left\{ (E_{i-1,j}^n + E_{i+1,j}^n - 2E_{i,j}^n) + (E_{i,j-1}^n + E_{i,j+1}^n - 2E_{i,j}^n) \right\} \quad (3.29)$$

Note that the space-time modulation is encoded in the space-time dependence of $\epsilon_{r_{i,j}}^n$. Next subsection discusses the method by which the amplitude and phase of the modulated sideband (harmonic) wavefronts are estimated and filtered out.

3.5.1 Phase sensitive detection of the modulated harmonic (sideband) wavefronts

The carrier light source is a continuous wave with temporal frequency ω_0 , propagating through a disordered medium and it interacts with a localised space-time modulated (STM) region within the wave propagation domain. The STM region acts as a travelling grating oscillating at a temporal modulation frequency, ω_{mod} and has the spatial modulation frequency, k_{mod} .²⁶ Due to the spatio-temporal interaction between the light wave and the STM region, the transmitted and the reflected waves contain different harmonic wavefront components having temporal frequencies $\dots, \omega_{-3} = \omega_0 - 3\omega_{mod}$, $\omega_{-2} = \omega_0 - 2\omega_{mod}$, $\omega_{-1} = \omega_0 - \omega_{mod}$,

26: For the STM modulations presented in the chapter $\omega_{mod} < \omega_0$ and $k_{mod} < k_{ref}$.

$\omega_{+1} = \omega_0 + \omega_{mod}$, $\omega_{+2} = \omega_0 + 2\omega_{mod}$, $\omega_{+3} = \omega_0 + 3\omega_{mod}$, etc.... Generally $\omega_{\pm n} = \omega_0 \pm n\omega_{mod}$ where the $\mathbf{n}$ (as a bold letter $\mathbf{n}$ to distinguish from the *FDTD* time stepping index n) denotes the temporal diffraction order number²⁷ involved in the *STM* modulation. For phase conjugating a particular modulated harmonic (side-band) wavefront, the amplitude and phase of that particular modulated wavefront, at a given $\mathbf{n}$ value, have to be determined. Such a phase sensitive detection scheme is given in [87] for seismic waves (for a multi-frequency scenario where there is a constant frequency separation ω_{mod} between various harmonics components). Let the multi-frequency transmitted wave be $E_{trans}(r, t)|_{\Gamma_R}$ evaluated at the transmitting boundary. Lets say that the amplitude and phase of the $\mathbf{n}^{th}$ modulated wavefront with temporal frequency $\omega_{\mathbf{n}} = \omega_0 + n\omega_{mod}$ has to be estimated. Let there be two reference signals oscillating at the $\mathbf{n}^{th}$ order temporal frequency such that,

$$\begin{aligned} E_{\mathbf{n}}^{ref_{0^\circ}} &= E_{ref} \cos(\omega_{\mathbf{n}} t + \theta_{ref}) \\ E_{\mathbf{n}}^{ref_{90^\circ}} &= E_{ref} \cos(\omega_{\mathbf{n}} t + \theta_{ref} + \pi/2) \end{aligned} \quad (3.30)$$

where $\omega_{\mathbf{n}} = \omega_0 + n\omega_{mod}$, $E_{\mathbf{n}}^{ref_{0^\circ}}$ is the in-phase reference signal at $\omega_{\mathbf{n}}$ and $E_{\mathbf{n}}^{ref_{90^\circ}}$ is the quadrature phase reference signal at $\omega_{\mathbf{n}}$ corresponding to the $\mathbf{n}^{th}$ harmonic frequency. In the implementation of the coding, the amplitude E_{ref} can be set to unity and the phase θ_{ref} to be zero, for convenience. Next step is to measure the spatially resolved temporal cross-correlation of the transmitted wave $E_{trans}(z, y, t)|_{(z,y) \in \Gamma_R}$, with that of the in-phase reference signal and the quadrature phase reference signal, over a time cycle where the time cycle is now the beating time period $t_{beat} = 2\pi/\omega_{mod}$.

Phase sensitive detection for the $\mathbf{n}^{th}$ order temporally modulated wavefront

$$\begin{aligned} X_{\mathbf{n}}^{corr}(z, y)|_{(z,y) \in \Gamma_R} &= \frac{1}{t_{beat}} \int_{t=t_0}^{t=t_0+t_{beat}} E_{\mathbf{n}}^{ref_{0^\circ}}(t) E_{trans}(z, y, t)|_{(z,y) \in \Gamma_R} dt \\ Y_{\mathbf{n}}^{corr}(z, y)|_{(z,y) \in \Gamma_R} &= \frac{1}{t_{beat}} \int_{t=t_0}^{t=t_0+t_{beat}} E_{\mathbf{n}}^{ref_{90^\circ}}(t) E_{trans}(z, y, t)|_{(z,y) \in \Gamma_{trans}} dt \end{aligned} \quad (3.31)$$

Then, the amplitude $E_{\mathbf{n}}^{trans}(z, y)|_{(z,y) \in \Gamma_R}$ and phase $\phi_{\mathbf{n}}^{trans}(z, y)|_{(z,y) \in \Gamma_R}$ of the $\mathbf{n}^{th}$ temporal component contained within the transmitted wave $E_{trans}(z, y, t)|_{(z,y) \in \Gamma_R}$ is reconstructed as the following

$$\begin{aligned} E_{\mathbf{n}}^{trans}(z, y)|_{(z,y) \in \Gamma_R} &= 2\sqrt{X_{\mathbf{n}}^{corr}(z, y)^2 + Y_{\mathbf{n}}^{corr}(z, y)^2}/E_{ref} \\ \phi_{\mathbf{n}}^{trans}(z, y)|_{(z,y) \in \Gamma_R} &= \tan^{-1}(Y_{\mathbf{n}}^{corr}(z, y)/X_{\mathbf{n}}^{corr}(z, y)) + \theta_{ref} \end{aligned} \quad (3.32)$$

Thus, the amplitude and phase of the $\mathbf{n}^{th}$ temporal component in the transmitted wave are estimated. Similarly, for the reflected wave, the amplitude and phase of the $\mathbf{n}^{th}$ sideband component are also estimated.

27: The temporal order number $\mathbf{n}$ is an integer due to the energy conservation principle involved in the interaction process between the *STM* region oscillating at a given monochromatic frequency ω_{mod} , and the carrier light wave at ω_0 .

[87]: Nihei et al. (2007), 'Frequency response modelling of seismic waves using finite difference time domain with phase sensitive detection (TD—PSD)'

3.5.2 Phase sensitive detection : Bragg vs Raman-Nath diffraction from a *STM* grating without any disorder present

In this chapter, for the space-time modulated (*STM*) grating, the time dependent relative dielectric permittivity constant $\epsilon_r(r, t)$ seen in the equation 3.1, takes a sinusoidal spatio-temporal modulation in the *STM* grating region as the following

$$\eta^2(r, t) = \epsilon_r(r, t) = \epsilon_r^{ref} + \delta\epsilon_r \{1 + \sin(k_{mod}y - \omega_{mod}t)\} \quad (3.33)$$

where ϵ_r^{ref} is the dielectric constant of the reference region surrounding the grating, $\delta\epsilon_r$ is the dielectric modulation amplitude, $k_{mod} = 2\pi/\Lambda$ is the *STM* spatial frequency, ω_{mod} is the *STM* temporal frequency and $\eta(r, t)$ is the refractive index. Let the average relative dielectric constant of the grating be denoted as $\epsilon_r^{avg} = \epsilon_r^{ref} + \delta\epsilon_r$. The diffraction from a space-time modulated grating is categorised into two main regimes,[82, 102] namely the Raman-Nath regime and the Bragg regime.²⁸ As there is no sharp or sudden step-change cross-over from one regime to another at a given fixed *STM* parameters, several works have been published with a goal to define a parameter to distinguish the two regimes of operation. Historically, an earlier popular choice was to use the Klein-Cook[103] parameter Q to broadly distinguish the regimes. Q is defined as the following

$$Q = \frac{k_{mod}^2 L}{k_{ref}} = \left(\frac{k_{mod}}{k_{ref}} \right) (k_{mod} L) = \frac{2\pi\lambda L}{\Lambda^2 n_{ref}} \quad (3.34)$$

where $k_{ref} = (2\pi\eta_{ref})/\lambda$ is the light spatial frequency, $k_{mod} = 2\pi/\Lambda$ is the *STM* spatial modulation frequency and L is the longitudinal thickness of the grating. For $Q > 10$ probability for being in the Bragg regime is high and on the other hand for Q of the order of unity or below, it is the Raman-Nath regime which is highly probable now. For the validity of the Klein-Cook parameter in identifying the operating regime to be Bragg or Raman-Nath, one more parameter ν has to be considered[103] as a constraint for capping the degree of modulation, while setting the *STM* parameters given in equation 3.34. It is recommended[103] to have $\nu < 6$, for the validity of the analysis involving the Q parameter where ν is given as

$$\nu = (k_{ref} L) \delta\epsilon_r \quad (3.35)$$

such that $\delta\epsilon$ is the peak dielectric constant modulation due to the *STM* grating. Based on the Q parameter, the operating regime of the *STM* region can be carefully tuned by selecting appropriate parameters associated with the carrier wave and the *STM* region. A detailed modelling study for that is given by Taravati and Eleftheriades[82], which is extended and generalised in this chapter by incorporating the phase sensitive detection (as shown in Figure 3.13(b) and (d)) and phase conjugation, to be made adaptable for wavefront shaping application needs in the disordered media. An example of such a tuning to choose between the Bragg regime and the Raman-Nath regime, without²⁹ any disorder present, is provided in Figure 3.13, where the parameters used are given

[102]: Moharam et al. (1978), 'Criterion for Bragg and Raman-Nath diffraction regimes'

[82]: Taravati et al. (2019), 'Generalized space-time-periodic diffraction gratings: Theory and applications'

[103]: Klein et al. (1967), 'Unified approach to ultrasonic light diffraction'

28: The Raman-Nath regime is occasionally referred as the thin-grating regime with a comparatively lower spatial modulation frequency. The Bragg regime is sometimes referred as thick-grating regime with a comparatively higher spatial modulation frequency. The Bragg regime is characterised by one or two spatial diffraction orders as shown in Figure 3.13(a) and the Raman-Nath regime is characterised by multiple spatial diffraction orders as shown in Figure 3.13(c).

29: The purpose of studying the *STM* grating response **without** any disorder present, is to validate and verify that the *STM* grating works as intended, as adding a disorder would scramble and mix various spatio-temporal diffraction orders. Disorder will be added later along with the *STM* grating operating in the Raman-Nath regime, for achieving the intended goals of this chapter.

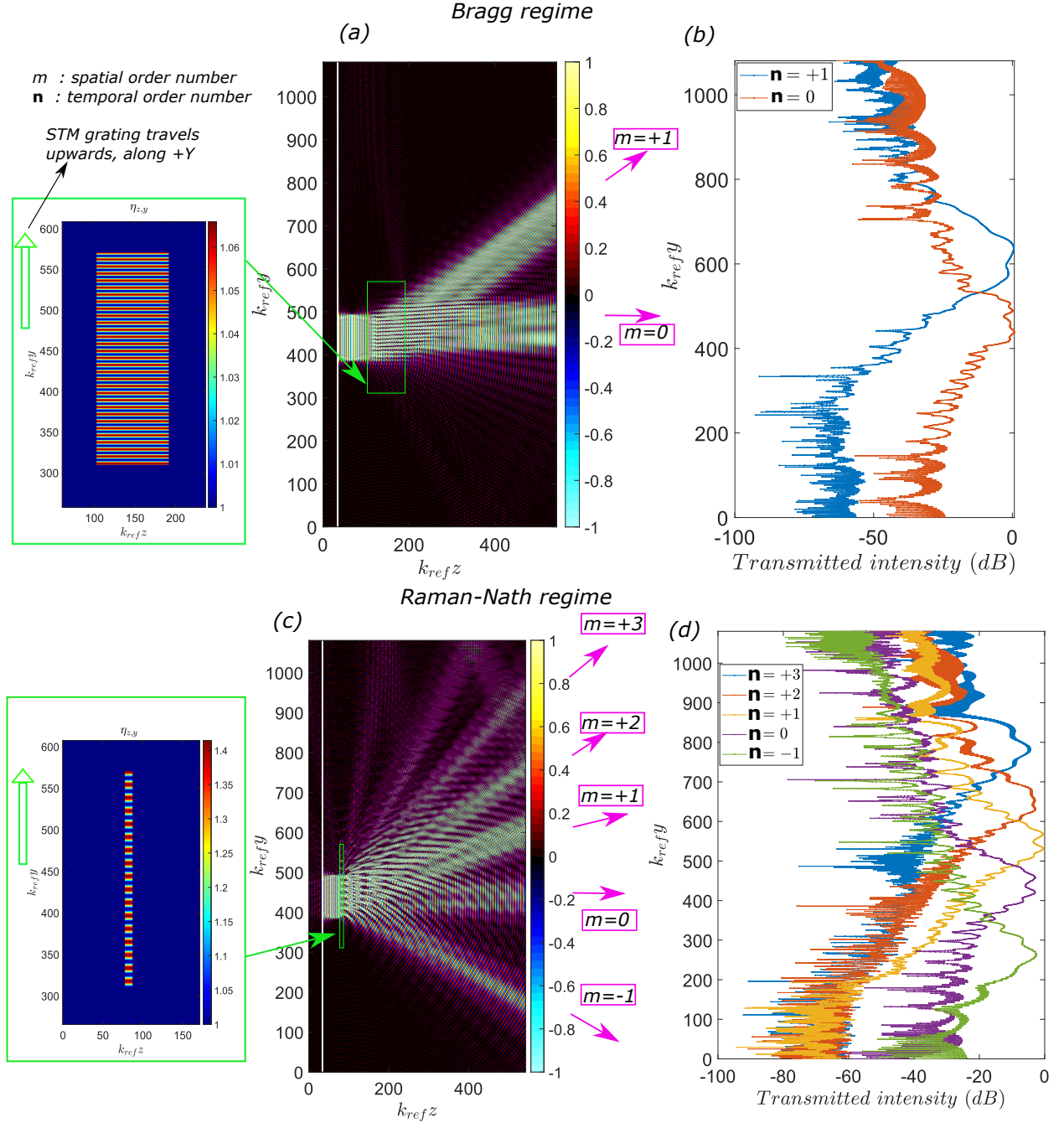


Figure 3.13: Phase sensitive detection scheme explained in Section 3.5.1 applied onto the spatio-temporal diffracted orders involved with the Bragg and the Raman-Nath regimes, without any disorder present. (a) The total field associated with the wave propagation involving a STM region (enclosed within the green box) operating in the Bragg regime is shown. Two spatial orders indexed by $m = 0$ and $m = +1$ are shown such that the STM modulation within the green box propagates upward along +Y axis. For the Bragg regime shown in here, $k_{mod}L = 64.21$ and $k_{ref}L = 87.9646$, where L is the longitudinal thickness (along z axis) of the STM region, $k_{mod}/k_{ref} = 0.73$, $\omega_{mod}/\omega_0 = 0.2$, Klein-Cook parameter $Q = 46.8763$ and $\nu = k_{ref}L\delta\epsilon_r = 5.982$ where $\delta\epsilon_r = 0.068$. (b) Phase sensitive detection of the temporally modulated wavefronts with temporal frequencies $\omega_n = \omega_0 + n\omega_{mod}$ is performed, where n is the temporal order number (represented as a bold letter n to distinguish from the FDTD time stepping index n). Both amplitude and phase of the modulated wavefronts are estimated and only the amplitude is plotted. (c) The total field associated with the Raman-Nath STM diffraction orders are shown. Here, there are multiple spatial diffraction orders indexed by m and the temporal diffraction orders are plotted in (d). For the Raman-Nath regime shown here, $k_{mod}L = 3.7196$ and $k_{ref}L = 9.2991$, $k_{mod}/k_{ref} = 0.4$, $\omega_{mod}/\omega_0 = 0.2$, Klein-Cook parameter $Q = 1.4879$ and $\nu = k_{ref}L\delta\epsilon_r = 4.6496$, where $\delta\epsilon_r = 0.5$. For both the Bragg and the Raman-Nath regimes, the STM grating takes the form given in equation 3.33, with a single temporal frequency component Ω_{mod} and a single spatial frequency component k_{mod} .

in the figure caption. In the Figure 3.13, various temporal diffraction orders are denoted by the index $\mathbf{n}$ and the spatial diffraction orders³⁰ by the index m . As the *STM* region is travelling (modulated) upwards along $+Y$, the interaction between the light wave and the *STM* grating causes the spatial diffraction orders of positive indices (where $m > 0$) to diffract upwards with respect to the zeroth ($m = 0$) spatial order. This is due to the momentum conservation of the interaction process, between the light wave and the *STM* wave. If the *STM* region was propagating downwards along $-Y$ direction, then the spatial orders seen before diffract downwards. For detecting the amplitude and the phase of the $\mathbf{n}^{th}$ modulated wavefront with the temporal frequency $\omega_0 + \mathbf{n}\omega_{mod}$, a phase sensitive lock-in detection scheme covered in Section 3.5.1 is employed.

In Figure 3.13, one may notice that for both the Bragg and the Raman-Nath gratings, there is only one single temporal frequency Ω_{mod} at which the *STM* gratings oscillate. In addition to that, there is also one single spatial frequency k_{mod} at which the *STM* gratings vary spatially along Y . Still, several temporal diffraction wavefront orders ($\mathbf{n} = \dots, -1, 0, +1, +2, +3, etc.$) are generated as shown in Figure 3.13(d), for the Raman-Nath regime. Also, it needs to be emphasised that, every spatial order would contain many temporal diffraction orders, but at different intensity levels. As an example, with respect to Figure 3.13(c) and (d), the $m = -1$ spatial diffraction order would contain the $\mathbf{n} = -1$ temporal diffraction order with temporal frequency ω_{-1} as its dominant component, but also contains the temporal orders $\mathbf{n} = 0, +1, 2, 3, ..etc.$ at weaker intensities in comparison with the $\mathbf{n} = -1$ order. After confirming (using Figure 3.13) that the *FDTD* coding for the *STM* grating is working as intended, disorder is added in the next section for using the *STM* grating in the Raman-Nath regime as a guide-star for phase conjugation applications.

30: One may notice that the spatial distribution of the diffraction pattern from the *STM* region has an asymmetric distribution around the $m = 0$ wavefront. This is mainly due to conservation of momentum involving the light wave momentum and the momentum due to the *STM* modulation which travels upwards along the $+Y$ axis. For further details, refer to [82].

3.6 Wavefront shaping in the Raman-Nath regime : Focussing onto a *STM* guide-star

Two kinds of phase conjugation involving the Raman-Nath *STM* grating given in Figure 3.13(c), but this time involving a disordered medium are shown. Case 1 is when the *STM* region is on the left side of the disorder as shown in the Figure 3.14(a), directly being excited by the incident beam. The modulated wavefronts then undergo multiple scattering through the disorder. The disorder has a transmission corresponding to the diffusion regime as given in the figure caption. The second case is when the *STM* region is surrounded by two disordered slab as shown in Figure 3.14(d), which operates in the diffusion-to-ballistic cross-over regime (Refer the figure caption for the transmission and the reflection value). An aspect to be noted is that during phase conjugation, the *STM* region is switched off.

3.6.1 Phase conjugation onto a *STM* guidestar

Using the phase sensitive detection scheme given in Section 3.5.1, the amplitude and the phase of the $\mathbf{n}^{th}$ modulated wavefront with the temporal frequency $\omega_0 + \mathbf{n}\omega_{mod}$ is estimated for the phase conjugation applications. Upon knowing the amplitude and phase of the desired temporal order to be phase conjugated, the same amplitude and phase of the wave can be assigned to an array of dipole sources (with the same temporal frequency of the modulated wavefront detected, ω_n) on the right side of the disorder. This is to phase conjugate the wave to be focussed on the *STM* region from where the modulated wavefronts originated. An incident beam larger than the *STM* region is used intentionally, to verify that the phase conjugated wave due to the modulated wavefronts converge back to the smaller *STM* region and not to the larger source region (especially for the case 1, where the *STM* region is on the left side of the disorder).

Both the wavefronts corresponding to $\mathbf{n} = +1$ (the upper sideband) and $\mathbf{n} = -1$ (the lower sideband), are phase conjugated separately as shown in the Figure 3.14(b) and Figure 3.14(c) respectively, to demonstrate the directionality³¹ of the phase conjugation involved. Figure 3.14 demonstrates the focussing through phase conjugation, involving the *STM* region placed in different relative positions with respect to the disorder. For the case shown in Figure 3.14 (e), the phase conjugate wave from the right reaches the *STM* region and then diverge to the left side of the *STM* region, to be scattered back to the interior region (between the two slabs) by the slab at the left side of the *STM* region. The two slabs also cause the *STM* modulated wavefronts to undergo multiple scattering in the interior region upon forward propagation. These two effects probably create the background intensity around the *STM* region within the interior region, upon phase conjugation. The two slabs and the transverse mirror boundary conditions forms a scattering cavity if the slabs are highly diffusive (in the deep diffusion regime, instead of the diffusion-to-ballistic cross-over regime taken for the example shown in Figure 3.14(d) and (e)). After observing the Figure 3.14, one could theorise the scope for tomography to focus light locally inside the disorder. The decorrelation of the sample (quantitatively explained in Section 3.4.1), sets up a temporal threshold time (given in Section 3.4.1) by which the phase conjugation has to be performed before the focus defocusses as shown in Figure 3.11. This section presented one time phase conjugation onto the *STM* region and the normalised intensity at the focus is given in Figure 3.14(f). For enhancing the contrast of focussing, iterative phase conjugation through a *STM* region will be discussed in Chapter 4.

31: In regards to the Figure 3.13, one could observe that the $\mathbf{n} = +1$ temporal order diffracts upwards during the forward propagation with respect to the $\mathbf{n} = 0$ temporal order, as the *STM* grating is travelling upwards along $+Y$. Therefore, one should expect that when the same temporal order $\mathbf{n} = +1$ is phase conjugated, it retraces the same direction from which the diffraction order was originally emerged. On the other hand, for the $\mathbf{n} = -1$ temporal order, it diffracted downwards from the *STM* region with respect to the $\mathbf{n} = 0$ order on the forward propagation. Hence, for the phase conjugation of $\mathbf{n} = -1$ temporal order, once again it retraces the same direction from which the modulated wavefront was originated. This is true, even in presence of disorder as seen in Figure 3.14(b) and (c).

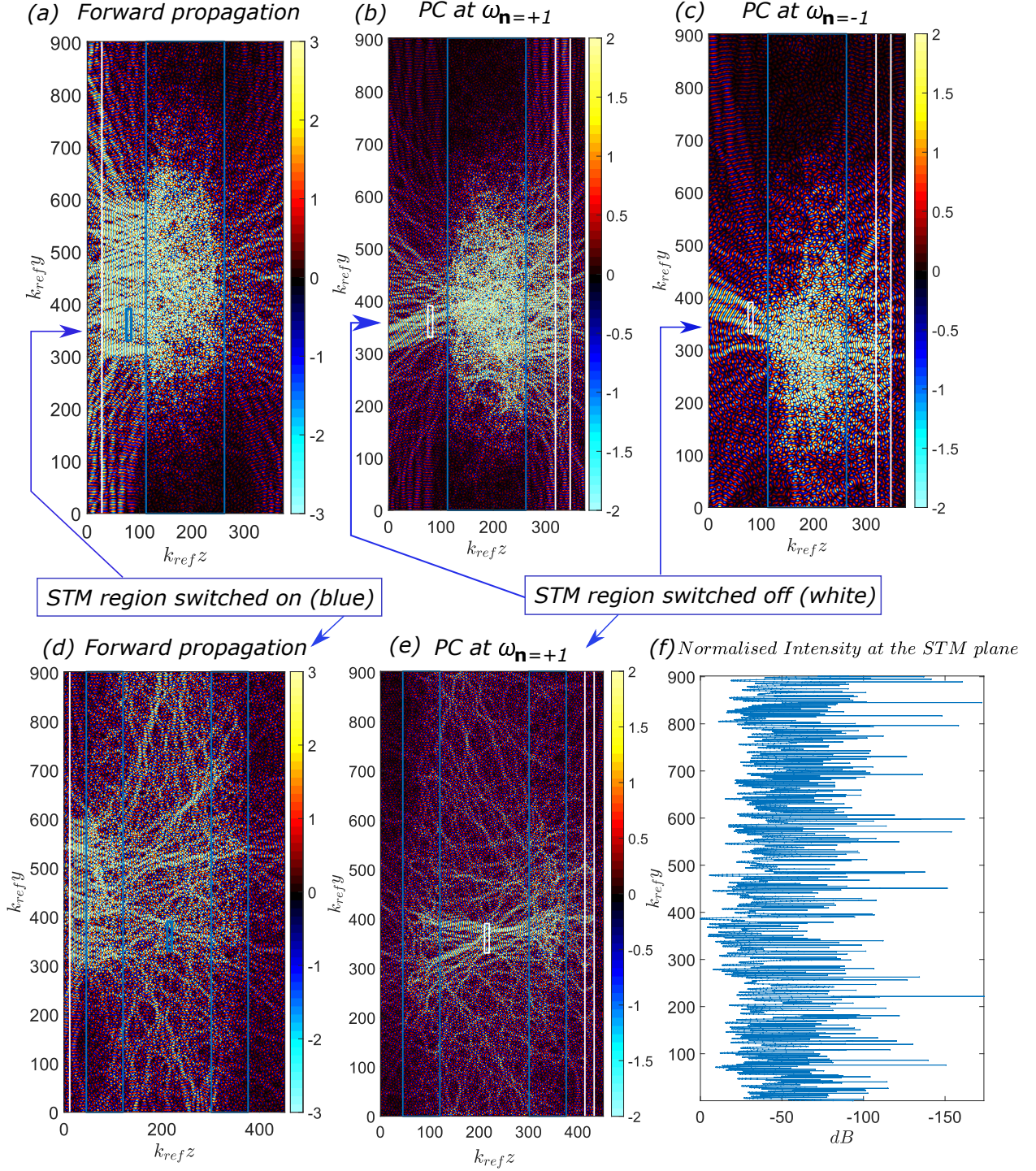


Figure 3.14: Forward propagation and phase conjugation (PC) involving an STM region operating in the Raman-Nath regime for two different geometries are shown. (a) Forward propagation at ω_0 is shown, where the incident beam directly excites the STM region (switched on, shown in blue colour, placed at the left side of the slab). Both the incident beam at ω_0 and the modulated wavefronts from the STM region, undergoes multiple scattering due to the disorder on the right. For the disorder without the STM region, $T = 0.17490$, $R = 0.81642$, $T + R = 0.99133$, therefore in the diffusion regime. (b) After phase sensitive detection of the $\omega_{n=+1}$ wavefront, it is phase conjugated at the same $\omega_{n=+1}$ frequency, to focus back at the STM location which is switched off (shown in white colour). $T = 0.58906$, $R = 0.41809$, $T + R = 1.00714$. (c) Similarly, the phase conjugation of the $\omega_{n=-1}$ wavefront at the same $\omega_{n=-1}$ frequency is shown, where $T = 0.66045$, $R = 0.32681$, $T + R = 0.98725$. (d) Forward propagation is shown, where the STM region (switched on, shown in blue colour, placed between two disordered slab). For the combination of the two disordered slabs, without the STM region switched on $T = 0.33453$, $R = 0.66692$, $T + R = 1.00145$, hence in the diffusion-to-ballistic cross over regime. (e) Phase conjugation of the $\omega_{n=+1}$ wavefront is shown at the same $\omega_{n=+1}$ frequency, where it attempts to focus back to the STM region such that $T = 0.56011$, $R = 0.43460$, $T + R = 0.99471$. (f) Intensity upon phase conjugation at the STM location is plotted for the case given in (e). Also, all the field plots have clipped colour map limits as shown, to make the focussing and background region visible with sufficient contrast.

3.7 Conclusion

The purpose of this chapter is to serve as an introduction to the *FDTD* formulation needed for modelling the wave transport phenomena in time domain. This is mainly to study the time dependent wavefront shaping phenomena such as the focussing using an *STM* guide-star and the effect of Brownian decorrelation on wavefront shaping. Studying these time dependent phenomena in the time domain was easier compared to the frequency domain methods, analytically and computationally. Hence, the change of direction from Chapter 1 (which described frequency domain methods) into the time domain methods presented in this chapter. Although the time domain method lacks the analytical depth in understanding the transport physics when compared to the frequency domain methods, the former is a valuable tool in exploring wavefront shaping aspects discussed in the chapter for a quicker and easier comprehension of the mentioned topics.

3.8 Future studies planned

A topic that is not explored in this chapter is the flux conservation when the *STM* region is under operation. All the results given in the chapter, where $R + T = 1$ is applicable for only those situations when the *STM* region is switch off while performing phase conjugation. The *STM* modulation performs work and adds energy onto the light scattering system. Maybe a generalised continuity equation needs to be incorporated to address the work done by the *STM* region onto the light wave. This is to address the total energy budgeting of the *STM* modulated system (to be explored in the future). Also, a potential work which could be explored in the future is to translate all the modelling explained in this chapter into the frequency domain. That will help to estimate the transmission matrix in presence of the *STM* region and estimate the eigenchannels through the *STM* region. To the best of my knowledge, only the experimentally obtained transmission matrix[4] in presence of the *STM* region has been published. The theoretical and the numerical investigation of such an acousto-optic transmission matrix is yet to appear in the literature.

Iterative phase conjugation in various wavefront shaping scenarios

4

4.1 Introduction

This chapter focusses on the modelling of the iterative phase conjugation phenomena for various wavefront shaping scenarios. The word “iterative” corresponds to the phase conjugation of the waves from the left and the right sides of the disorder, sequentially, starting from an unshaped wave incidence to converge upon a limiting behaviour of interest after several round trips. The limiting wave transport behaviour of interest in this chapter, upon iterative phase conjugation, is regarding the spatially constricted transport inside the disorder. The significance of such an iterative process is two fold. The first aspect is regarding the reason that the measurement of the transmission matrix is a time consuming process. The transmission matrix measurement also requires the medium to be stationary for a period of the full probing of the entire transmission matrix, to access the eigenchannels of the system. Iterative phase conjugation is comparatively a faster process and has the potential to access the maximally transmitted eigenchannel as modelled in this chapter. The second aspect is to increase the flux transport through a given region inside a disorder by the iterative phase conjugation method, in comparison to the one-time phase conjugation method given towards the end of Chapter 3. In the context of the experimental iterative phase conjugation, there are works published in acousto-optics[29, 104] and ultrasonics[105] for focussing applications. This chapter mainly focusses on the transmission enhancement and enhancing the focussing contrast attained inside a disorder, due to the iterative phase conjugation operation.

In the first half of the chapter, the iterative phase conjugation involving a dielectric aperture (with an opening) with a disorder placed around the aperture, is studied. Such a study is done using the frequency domain model developed in Chapter 1 which includes the estimation of the S matrix. This is followed by the study of the iterative phase conjugation involving a space time modulated (STM) guide-star region operating in the Raman-Nath regime surrounded by a disordered region. Such a study involves the methods introduced in Chapter 3. Both the first half and the second half of the chapter, deals with the effects of attaining coherent control of waves inside¹ the medium.

In the following section, the relation between the iterative phase conjugation and eigenchannels is explored. This would help to validate the expected results due to iterative phase conjugation, by comparing it with the maximally transmitting eigenchannel.

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- [29]: Si et al. (2012), ‘Breaking the spatial resolution barrier via iterative sound-light interaction in deep tissue microscopy’
[104]: Ruan et al. (2014), ‘Iterative time-reversed ultrasonically encoded light focusing in backscattering mode’

- [105]: Prada et al. (1991), ‘The iterative time reversal mirror: A solution to self-focusing in the pulse echo mode’

1: It needs to be emphasised that the main objective of this chapter is regarding the enhancement of the total transmission out of a disorder, while constricting the flow through a specified region inside the disorder. Such an objective of enhancing the total transmission through a region, doesn’t guarantee to converge upon a wave solution that create a high intensity focus, localised around the interested region inside the disorder. That is mainly because the objective is to optimise the total transmission constricted through a region and not to obtain the largest intensity or focussing contrast at the region. There could exist a wave hypothetically, that focusses well on the constricting region inside the disorder, creating a large intensity or focussing contrast, but doesn’t transmit well out of the second half of the disorder.

4.2 Relation between iterative phase conjugation and eigenchannels

The relation between iterative phase conjugation and eigenchannels is given in supplementary material of Katz et al [4] in the context of the acousto-optic transmission matrix. Such a relation is generalised in this section to include the gain factors. In addition to that, in this section the equivalence between the maximally transmitting eigenchannel and iterative phase conjugation is numerically validated using the frequency model defined in Chapter 1 without including the *STM* modulation. Let c_{inc}^{rand} be the modal coefficients of a random arbitrary wave incident on the medium from the left to the right side of the disorder. As discussed in Chapter 1, c_{inc}^{rand} denotes the eigenmode basis expansion coefficients² of the incident wave. Such a random wave to start the iterative phase conjugation process, is flux normalised such that the flux injected by the incident wave (without the disorder or the aperture) is unity. Then, the transmitted wave at the right side of the disorder is given as

$$c_{trans1} = S_{21}^{prop,prop} c_{inc}^{rand} \quad (4.3)$$

where $S_{21}^{prop,prop}$ is the propagating part,³ of the transmission matrix due to the wave transmission from the left to the right side of the disorder and c_{trans1} contains the modal coefficients of the transmitted wave. Let the modal coefficients of the transmitted wave represented by c_{trans1} , be phase conjugated with a multiplicative gain g_2 (a scalar real number multiplied onto the phase conjugated field value) from the right side of the disorder. The gain factor g_2 is normalised such that the flux injected by the phase conjugate wave from the right side of the disorder (without any scattering) is unity. Then the phase conjugated wave before entering the medium from the right side of the disorder is represented as $c_{pc1} = g_2 c_{trans1}^*$, where $*$ denotes complex conjugation operation for the phase conjugation. Then, using equation 4.3 the transmitted wave through the medium from the right side to the left of the disorder is given as

$$\begin{aligned} c_{trans2} &= S_{12}^{prop,prop} c_{pc1} \\ &= S_{12}^{prop,prop} (g_2 c_{trans1}^*) \\ &= S_{12}^{prop,prop} (g_2 (S_{21}^{prop,prop} c_{inc}^{rand})^*) \end{aligned} \quad (4.4)$$

where $S_{12}^{prop,prop}$ is the transmission matrix for waves incident from the right side to the left of the disorder. Due to the reciprocity principle⁴ for the propagating modes, $S_{12}^{prop,prop} = \{S_{21}^{prop,prop}\}^T$. Therefore

$$\begin{aligned} c_{trans2} &= S_{12}^{prop,prop} (g_2 (S_{21}^{prop,prop} c_{inc}^{rand})^*) \\ &= \{S_{21}^{prop,prop}\}^T (g_2 (S_{21}^{prop,prop} c_{inc}^{rand})^*) \\ &= g_2 \{S_{21}^{prop,prop}\}^T (S_{21}^{prop,prop} c_{inc}^{rand})^* \end{aligned} \quad (4.5)$$

The next step is to phase conjugate c_{trans2} with a scalar gain factor g_1 such that the influx injected from the left side upon phase conjugation is

[4]: Katz et al. (2019), ‘Controlling light in complex media beyond the acoustic diffraction-limit using the acousto-optic transmission matrix’

2: As given in equation 1.60, the random incident wave can be expanded in the eigenmode basis as,

$$\tilde{E}_{inc}^{rand}(z, y)|_{(z,y) \in \Gamma_L} = \sum_{m=1}^{M_{total}} c_{rand,m}^+ \chi_m(y) \phi_m^+(z) \quad (4.1)$$

such that,

$$c_{inc}^{rand} = (c_{rand,1}^+, c_{rand,2}^+, c_{rand,3}^+, \dots, c_{rand,M_{prop}}^+)^T \quad (4.2)$$

3: Refer the first row of the table 1.2, for the evaluation of the matrix elements representing the propagating part of the S_{21} , where both the incident and the transmitted modes, are propagating.

4: The reciprocity principle involving the propagating modes is explained towards the end of Section 1.5.5 in Chapter 1.

again unity. This completes one round trip to obtain

$$\begin{aligned} c_{pc2} &= g_1 c_{trans2}^* \\ &= g_1 \left(g_2 \{S_{21}^{prop,prop}\}^T (S_{21}^{prop,prop} c_{inc}^{rand})^* \right)^* \\ &= g_1 g_2 \{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop} c_{inc}^{rand} \end{aligned} \quad (4.6)$$

where $\dagger$ denotes the Hermitian conjugate. The term $\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop}$ is usually referred to as the time reversal operator[106]. Here, one round trip consists of two phase conjugations and two transmissions through the random medium as given in[4]. For the purpose of plotting, g_1 and g_2 can be combined into a single term $g_1^{IPC} = g_1 g_2$, where the subscript *IPC* stands for iterative phase conjugation. After k number of round trips, the incident phase conjugate wave is represented as the outcome of the following limiting scattering behaviour

Iterative phase conjugation (IPC) profile after k roundtrips

$$c_k^{pc} = g_1^{IPC} g_2^{IPC} g_3^{IPC} \dots g_k^{IPC} \left(\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop} \right)^k c_{inc}^{rand} \quad (4.7)$$

where $g_1^{IPC} = g_1 g_2$, $g_2^{IPC} = g_3 g_4$, $g_3^{IPC} = g_5 g_6$ etc...⁵

As explained in Chapter 1, any wave that exist in the computational domain can be represented in two different basis space. The first being the eigenmode basis space and the second being the eigenchannel basis space. As c_{inc}^{rand} was represented in the eigenmode basis space, the coefficients c_{inc}^{rand} is transformed into the eigenchannel basis space, by using the singular column vectors V involved with the singular value decomposition ($S.V.D$) of the $S_{21}^{prop,prop}$ matrix. Therefore c_{inc}^{rand} could be represented in terms of d_{inc}^{rand} in the eigenchannel basis[4] of the $S_{21}^{prop,prop}$ matrix as given below

$$c_{inc}^{rand} = V d_{inc}^{rand} \quad (4.8)$$

where V is the matrix obtained from the $S.V.D$ ⁶ of $S_{21}^{prop,prop}$ such that, $U \Sigma V^\dagger = S_{21}^{prop,prop}$ as given in Chapter 1. The flux normalisation is represented as ($\|c_{inc}^{rand}\|_{L_2} = \|V d_{inc}^{rand}\|_{L_2} = 1$), where the L_2 norm of the coefficients is unity. Therefore,

$$\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop} V = [\tau] V \quad (4.9)$$

as V contains the eigenvectors for $\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop}$ and $[\tau]$, the corresponding eigenvalue diagonal matrix. Therefore, combining equations 4.7, 4.8 and 4.9, the following is obtained when k approaches a

[106]: Prada et al. (1994), 'Eigenmodes of the time reversal operator: A solution to selective focusing in multiple-target media'

[4]: Katz et al. (2019), 'Controlling light in complex media beyond the acoustic diffraction-limit using the acousto-optic transmission matrix'

5: The significance of the gain terms $g_1^{IPC} = g_1 g_2$, $g_2^{IPC} = g_3 g_4$, $g_3^{IPC} = g_5 g_6$, etc... is to balance the transmission loss (due to the reflectance on propagation) associated with iterative phase conjugation term $\left(\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop} \right)^k$, so that the flux injected in every wave incidence step is unity.

6: Σ is a diagonal matrix containing the singular values, which are the square roots of eigenvalues of $\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop}$ or $S_{21}^{prop,prop} \{S_{21}^{prop,prop}\}^\dagger$. The right singular vectors V of $S_{21}^{prop,prop}$ is the eigenvector for $\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop}$. Usually, the transmission coefficient matrix for eigenchannels is given as $[\tau] = \Sigma^2$ or Σ could be represented as $\Sigma = \sqrt{[\tau]}$, which is once again a diagonal matrix represented in terms of square root of eigenchannel transmission coefficients. The diagonal elements of Σ are usually ordered as $\sqrt{\tau_1} > \sqrt{\tau_2} > \sqrt{\tau_3}$ etc...

large number

$$\begin{aligned}
c_{limiting}^{pc} &= \lim_{k \rightarrow \infty} g_1^{IPC} g_2^{IPC} g_3^{IPC} \dots g_k^{IPC} \left(\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop} \right)^k c_{inc}^{rand} \\
&= \lim_{k \rightarrow \infty} g_1^{IPC} g_2^{IPC} g_3^{IPC} \dots g_k^{IPC} \left(\{S_{21}^{prop,prop}\}^\dagger S_{21}^{prop,prop} \right)^k V d_{inc}^{rand} \\
&= \lim_{k \rightarrow \infty} g_1^{IPC} g_2^{IPC} g_3^{IPC} \dots g_k^{IPC} [\tau]^k V d_{inc}^{rand}
\end{aligned} \tag{4.10}$$

The above given equation can be interpreted as given in the side note.⁷

After a large number of round trips ($k \rightarrow \infty$), the iteration would converge into the limiting field profile represented by the maximum transmitting eigenchannel (whose transmission coefficient is $\tau_{max} = \tau_1$), upon tuning the gain terms to obey the flux conservation equations, given in the side note. The maximally transmitting eigenchannel and the associated transmission coefficient, backed up by the gain terms becomes the convergent solution upon iterative phase conjugation. All the other eigenchannel modes with transmission coefficients $\tau_2, \tau_3, \dots < \tau_1 = \tau_{max}$, eventually loses out in the mode competition for survival, when a large number of round trips is achieved. For performing iterative phase conjugation (which includes the visualisation of the total field and the estimation of the total transmissions), the S matrix will be evaluated as per Chapter 1. This is mainly to access the S_{21} and S_{12} matrices contained within the S matrix.

4.3 S matrix, eigenchannels and iterative phase conjugation, for a disordered constricting aperture

In the following section, the evaluation of the S matrix for a dielectric⁸ aperture, without any disorder present in the computational domain, is demonstrated. Once the S matrix is evaluated, the transmission eigenchannels of $S_{21}^{prop,prop}$ and $S_{12}^{prop,prop}$ can be estimated. Such an analysis is followed by the addition of disorder around the aperture to constrict the multiply scattered waves through the aperture opening.

7: The incident waves from the left and the right sides of the disorder, is always flux normalised to inject unit flux (the transmission without the disorder due to the incident wave is unity). Therefore,

$$\|V d_{inc}^{rand}\|_{L_2} = 1 \tag{4.11}$$

$$\|g_1^{IPC} [\tau]^1 V d_{inc}^{rand}\|_{L_2} = 1 \tag{4.12}$$

$$\|g_1^{IPC} g_2^{IPC} [\tau]^2 V d_{inc}^{rand}\|_{L_2} = 1, \text{ etc...} \tag{4.13}$$

where $[\tau] = \text{diag}(\tau_1, \tau_2, \tau_3, \dots)$, diag represents a diagonal matrix and $\tau_1 = \tau_{max} > \tau_2 > \tau_3, \dots$ the diagonal elements. Therefore, effectively the gain terms get multiplied onto the diagonal matrix elements. The largest term in $g_1^{IPC} g_2^{IPC} g_k^{IPC} [\tau]^k$ is $g_1^{IPC} g_2^{IPC} g_k^{IPC} (\tau_{max})^k$, which gets naturally dominant when k becomes a large number. Hence the first eigenvector column of V , corresponding to $\tau_1 = \tau_{max}$, dominates, resulting in the transmission profile corresponding to the maximally transmitted eigenchannel.

8: The aperture is made of dielectric material with large dielectric constant value to act as a non-absorbing but reflecting surface. This ensures flux conservation such that, $T + R = 1$.

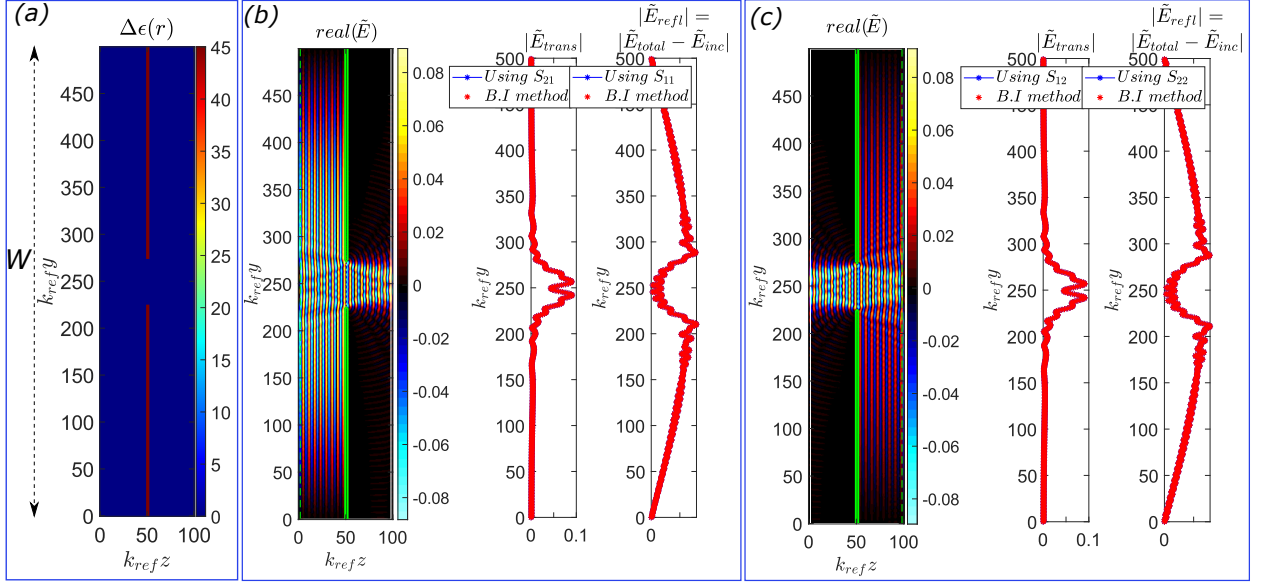


Figure 4.1: Geometry of the dielectric aperture and the total-field/scatter field (TF/SF) representation of the field due to the wave incidence, from the left and the right side of the aperture, are shown. (a) The disorder dielectric constant perturbation value $\Delta\epsilon_r(r)$ is given. For the aperture, $\Delta\epsilon_r(r) = 45$, against a uniform background refractive index $\eta_{ref} = 1.9$. $W/D_{apert} = 10$ where D_{apert} is the size of the aperture opening. **(b)** The diffraction of the aperture due to the first eigenmode of the computational domain without the aperture, incident from the left is given where $T = 0.1953$ and $R = 0.8047$. The aperture is enclosed in the green solid-dash boundaries and the TF/SF boundary is represented using green dashed lines. **(c)** Similarly, the diffraction of the aperture due to the first eigenmode of the computational domain without the aperture, incident from the right is shown where $T = 0.1953$ and $R = 0.8047$ is the same as before.

4.3.1 An aperture with an opening without any disorder

Figure 4.1(a) shows the geometry of the dielectric aperture used where a large dielectric constant perturbation value of 45 is taken. Figure 4.1(b) and (c) shows how the first eigenmode of the computational region without the aperture would be diffracted by the aperture, if the mode incidence is from the left side and the right side of the disorder, respectively. For many of such incident eigenmodes incident on the aperture, the S matrix can be evaluated using the same methods given in Chapter 1. The estimated S_{21} matrix is shown in Figure 4.2. The $S.V.D$ of the S_{21} matrix is used to estimate the transmission eigenchannels of the disorderless aperture as shown in Figure 4.3. The eigenchannel transmission coefficients τ for various eigenchannels through the aperture is given in Figure 4.4. The shown eigenchannel transmission coefficients consists of either highly transmitting or reflecting ones, with a step like change in between.

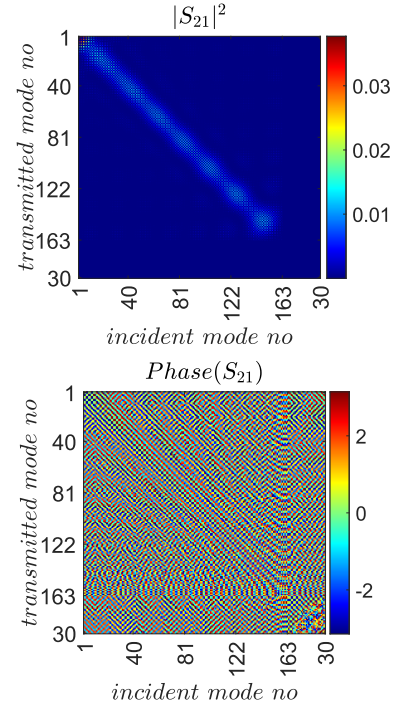


Figure 4.2: S_{21} for an aperture with an opening without any disorder.. (a) The magnitude and **(b)** the phase of the S_{21} matrix, of the disorderless aperture shown in Figure 4.1, are given.

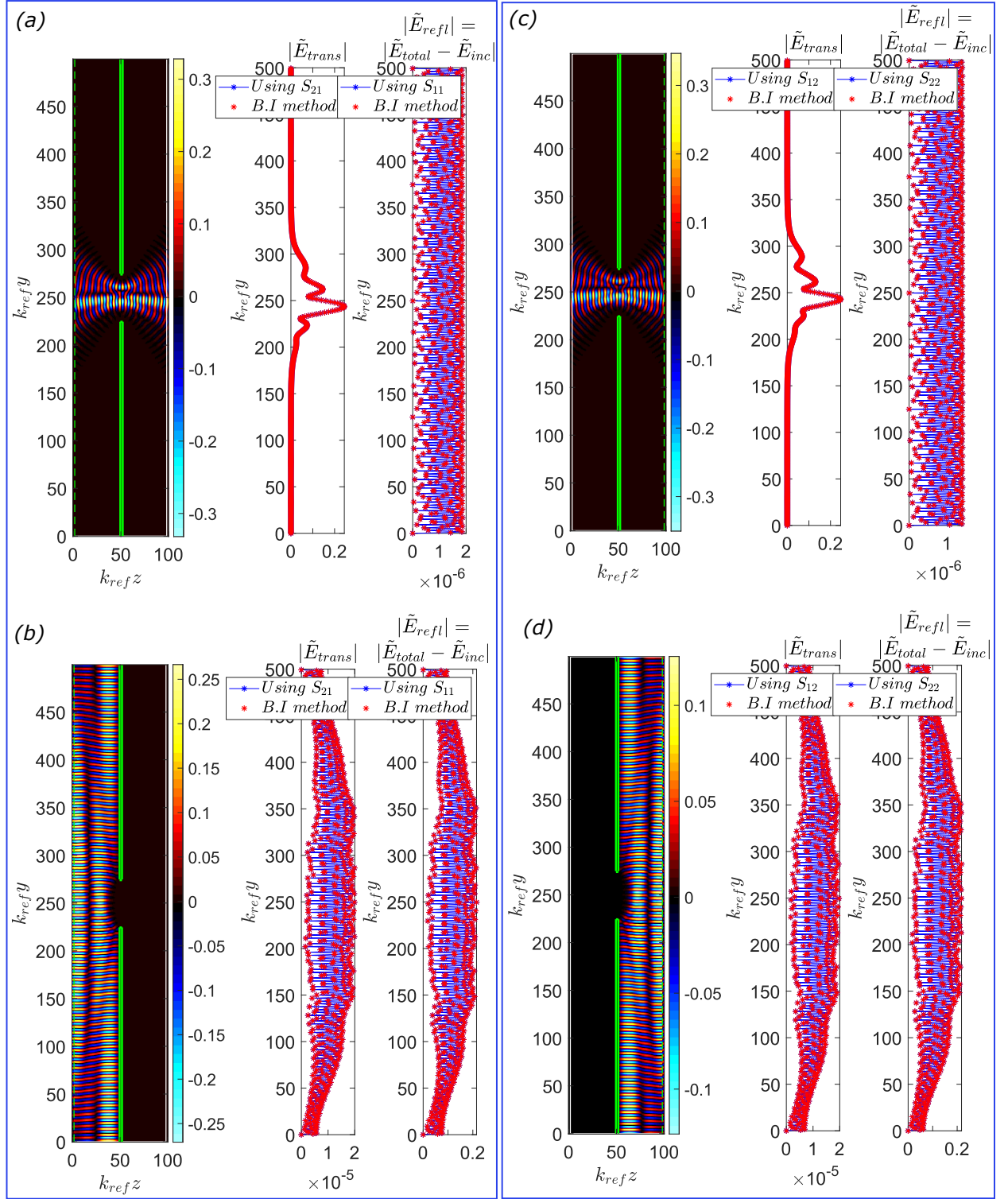


Figure 4.3: Maximally and minimally transmitting eigenchannels of $S_{21}^{prop,prop}$ and $S_{12}^{prop,prop}$ through a dielectric aperture without any disorder, are given. (a) Maximally transmitting eigenchannel of $S_{21}^{prop,prop}$, where $T = 1, R = 0$. (b) Minimally transmitting eigenchannel of $S_{21}^{prop,prop}$, where $T = 0, R = 1$. Similarly, (c) Maximally transmitting eigenchannel of $S_{12}^{prop,prop}$, where $T = 1, R = 0$. (d) Minimally transmitting eigenchannel of $S_{12}^{prop,prop}$, where $T = 0, R = 1$. The maximally transmitting eigenchannels of S_{21} and S_{12} looks alike with each other because, the transport path with the maximal transmission from the left to the right, would be the same path taken from the right to the left, to attain the same maximal transmission.

As shown in the Figure 4.3(a) and (c), the maximally transmitting eigenchannel transmits through the constriction opening as expected, without getting back-scattered. Similarly, the minimally transmitting eigenchannel gets reflected from the scattering part of the dielectric aperture and also from the transverse reflecting boundaries, as shown in the Figure 4.3(b) and (d). The maximally transmitting transport path from the left to the right of the aperture shown in Figure 4.3(a), would be the same path taken by the maximally transmitting transport path from the right to the left, shown in Figure 4.3(c).

4.3.2 A disordered constricting aperture

Upon seeing that the eigenchannels have the expected transport behaviour through the aperture, disorder can be added surrounding the aperture to model a constricted transport of multiply scattered waves. The wave transport geometry of such a constricted disordered aperture is shown in Figure 4.5.

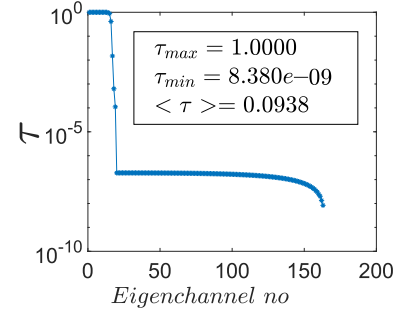


Figure 4.4: The transmission coefficients of the eigenchannels through an aperture opening, without any disorder is shown. The eigenchannel coefficients corresponds to the transmission matrix shown in Figure 4.2.

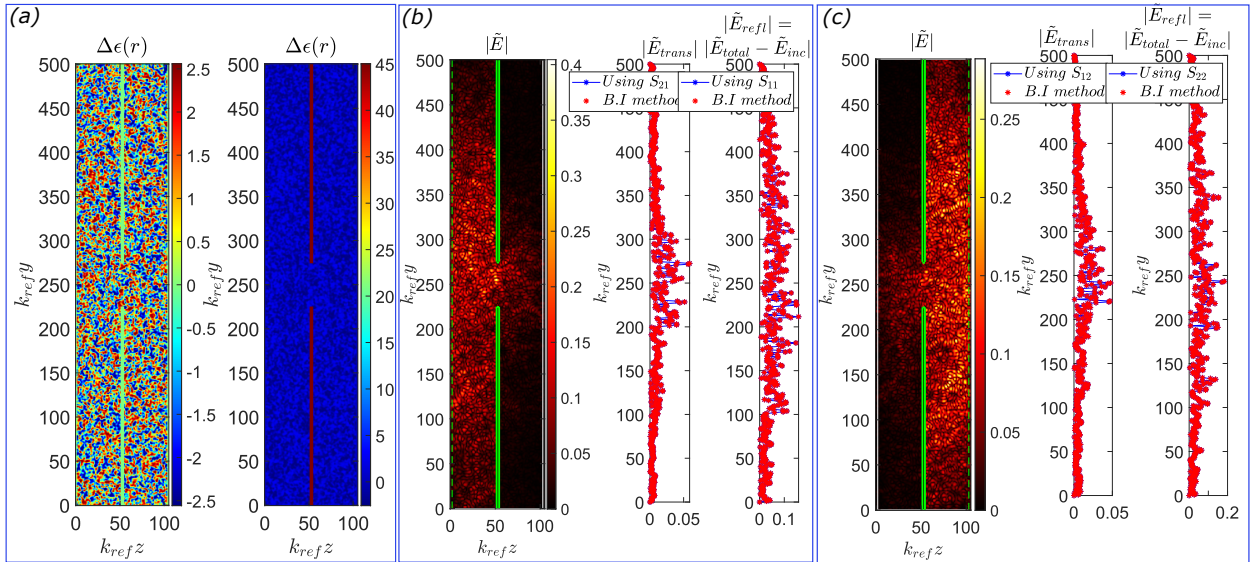


Figure 4.5: Geometry of the disordered constricting aperture used and the scattering response of the first eigenmode incident from the left and the right side, are demonstrated. (a) The disorder dielectric constant perturbation value, $\Delta\epsilon(r)$ is shown. On the left, just the disordered region without the aperture is shown. On the right, the aperture region with a high dielectric constant value of 45, is added onto the disorder shown on the left. The disorder shown on the left is in the diffusion regime and has the same properties as given in Figure 1.9 of Chapter 1. (b) The total-field/scatter field (TF/SF) in the disordered aperture, when the first eigenmode of the computational domain without the disorder excites from the left side is shown. $T = 0.0636$ and $R = 0.9364$. (c) Similarly, the TF/SF for the disordered aperture, when the first eigenmode of the computational domain without the disorder excites from the right side. $T = 0.0448$ and $R = 0.9552$.

4.3.3 Eigenchannels through a disordered constricting aperture

Similar to that of Section 4.3.1, the S matrix of the disordered constricting aperture given in Figure 4.9 is evaluated. Following that, the $S.V.D$ of the transmission matrix $S_{21}^{prop,prop}$ is evaluated to estimate the eigenchannels. The S_{21} matrix of the disordered constricting aperture is given in Figure 4.6(a) and (b) and the corresponding eigenchannel transmission coefficients are plotted in Figure 4.6(c). The magnitude profiles of various eigenchannels estimated are shown in Figure 4.7. Similar to that of

Section 4.3.1, the maximum transmitting eigenchannel of $S_{21}^{prop,prop}$ and $S_{12}^{prop,prop}$, have similar transport profiles because of the same reason that the largest transmitting transport path from left to right of the disorder, would be the same path from the right to the left as well. Such a similarity in the maximum transmitting eigenchannel from the left and the right, is also in agreement with the reason for the convergence of the magnitude profile inside the disorder during iterative phase conjugation when the iteration number becomes large enough, as demonstrated in the next section.

4.3.4 Iterative phase conjugation through a disordered constricting aperture

In this section, the equivalence between iterative phase conjugation with the gain factors and the maximally transmitted eigenchannel, is numerically demonstrated using the frequency domain models presented in Chapter 1. Figure 4.8 shows the iterative phase conjugation operation starting from a random unshaped wavefront obtained by a random c_{inc}^{rand} coefficient array. To begin with, the random wave is incident on the left side of the dielectric aperture (shown in Figure 4.8(a)), followed by the phase conjugation from the right (shown in Figure 4.8(b)). This is followed by one more phase conjugation on the left, before getting incident on the disordered aperture to complete one round trip. In other words, a round trip consists of 1) a transmission from left to right, 2) a phase conjugation operation on the right, 3) a transmission from right to left and 4) a phase conjugation on the left. Such an iterative phase conjugation process with many iterations are shown in Figure 4.8(e) to (h).

The increase in the total transmission during the iterative phase conjugation process and the eventual convergence onto the same transmission value of 0.9899 associated with the maximally transmitted eigenchannel, is plotted in Figure 4.9(a). The gain factors g^{IPC} taken during the iterative phase conjugation process, to selectively filter the mode resembling the maximally transmitting eigenchannel, is plotted in Figure 4.9(b), as a function of the number of round trips. It can be seen that the gain reduces and saturates to a constant value during the progress of the iterative phase conjugation process. To compare the converged magnitude profile inside the disordered region during the iterative phase conjugation process (shown in Figure 4.9(c)), with that of the maximally transmitting eigenchannel from the left (Figure 4.9(d)), the two magnitude profiles are subtracted and plotted in Figure 4.9(e) to show the small difference⁹ in the magnitude.

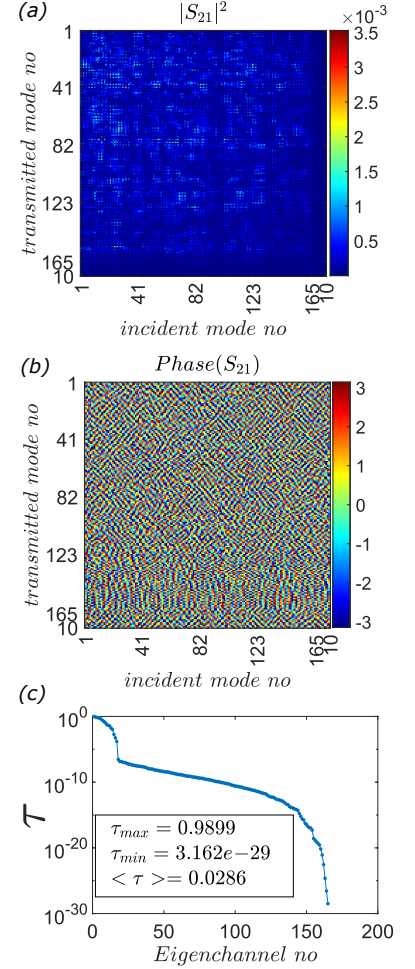


Figure 4.6: (a) The magnitude and (b) the phase of the S_{21} matrix and (c) the transmission coefficients of the eigenchannels through an aperture opening, in presence of disorder are shown.

9: The magnitude of the difference is small (10^{-9}) when compared to the magnitude of the fields (of the order of unity), which confirm that the iterative phase conjugation process converges towards the maximally transmitted eigenchannel.

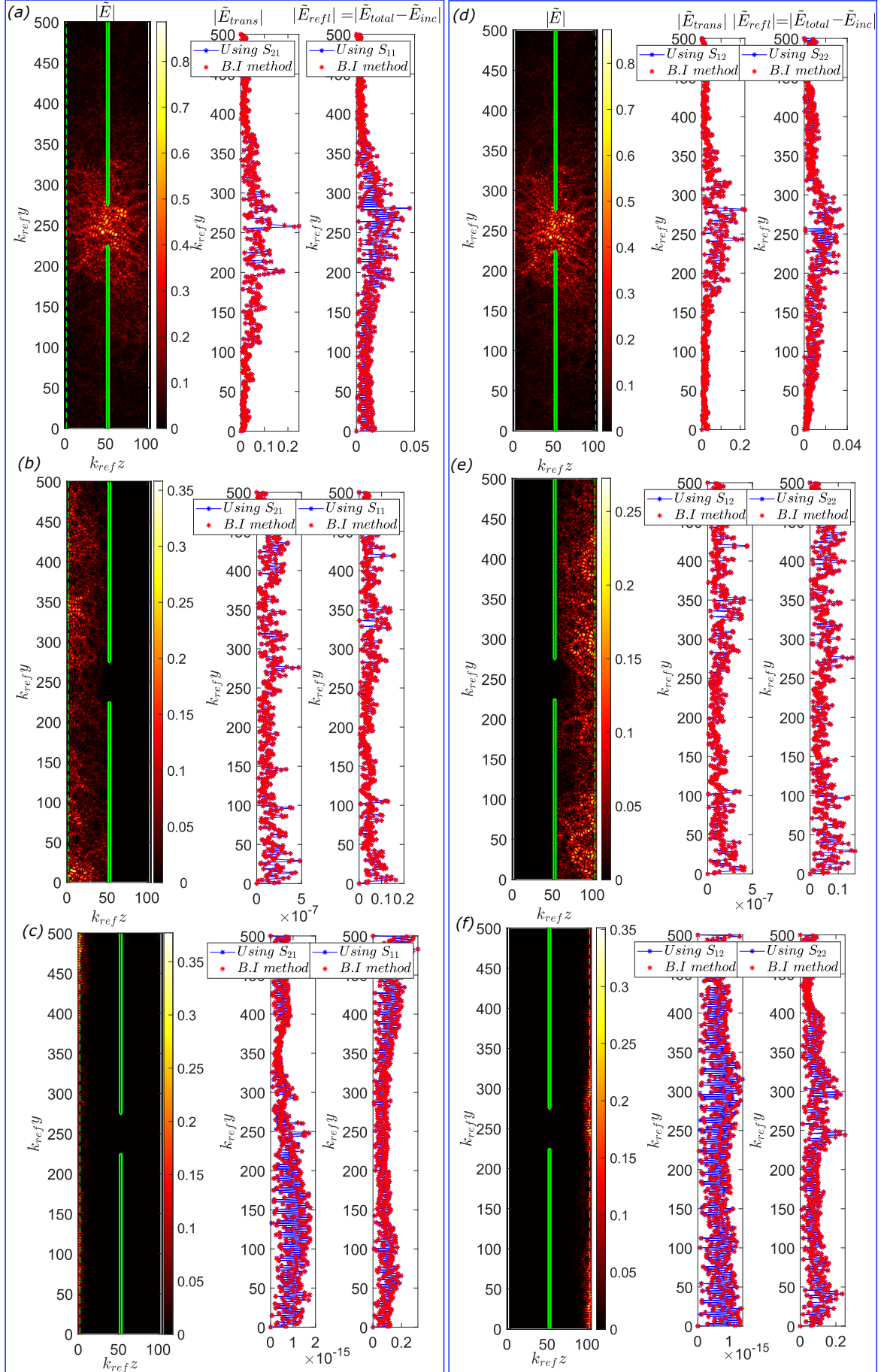


Figure 4.7: Various eigenchannels of S_{21} and S_{12} through a dielectric aperture in presence of disorder are shown. (a) Maximally transmitted (first) eigenchannel of S_{21} , where $T = 0.9899$ and $R = 0.0101$ (b) An intermediate eigenchannel numbered 110 out of the 165 eigenchannel modes of S_{21} where $T = 8.1842 \times 10^{-12}$. (c) Minimally transmitted (last eigenchannel numbered 165) eigenchannel of S_{21} , where $T = 3.1620 \times 10^{-29}$. Similarly, (d) Maximally transmitted (first) eigenchannel of S_{12} , where $T = 0.9899$, $R = 0.0101$. (e) An intermediate eigenchannel numbered 110 out of the 165 eigenchannel modes of S_{12} where $T = 8.1842 \times 10^{-12}$. (f) Minimally transmitted (last eigenchannel, numbered 165) eigenchannel of S_{12} where $T = 3.1350 \times 10^{-29}$.

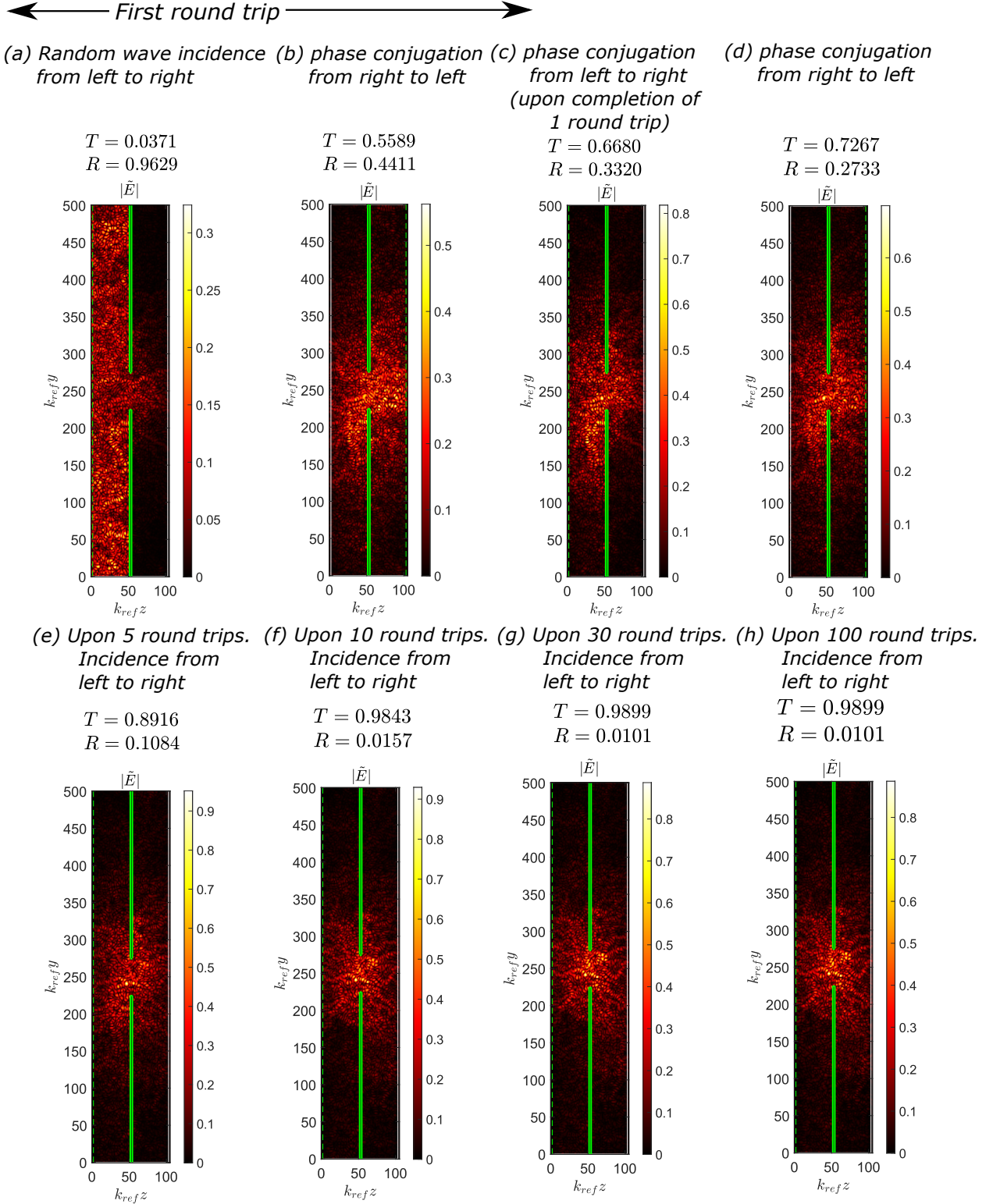


Figure 4.8: Magnitude of the total-field/scatter field associated with various roundtrips during the iterative phase conjugation through a constricting aperture surrounded by disorder, are shown. (a) The iterative phase conjugation method starts from a randomly initialised wave incident on the disorder with an embedded dielectric aperture, from the left. **(b)** The transmitted profile on the right is phase conjugated from the right side, to be emerging on the left side of the disorder. **(c)** The wavefront emerged on the left is phase conjugated again, to complete the first round trip. The scattering response after the completion of one round trip is shown. **(d)** The transmitted wave is phase conjugated from the right side. The process is repeated to demonstrate the magnitude profile after **(e)** 5 round trips, **(f)** 10 round trips, **(g)** 30 round trips and **(h)** 100 round trips. All the associated transmission and reflection values are given along with the magnitude profiles. As discussed in the chapter, the magnitude profile converges to that of the same magnitude profile associated with the maximally transmitted eigenchannel given in Figure 4.9(a). For the numerical comparison between the converged iterative phase conjugation profile with that of the maximum transmitted eigenchannel, refer Figure 4.9(c),(d) and (e). The complete profile for the total transmission and the gain taken, are provided in Figure 4.9(a) and (b).

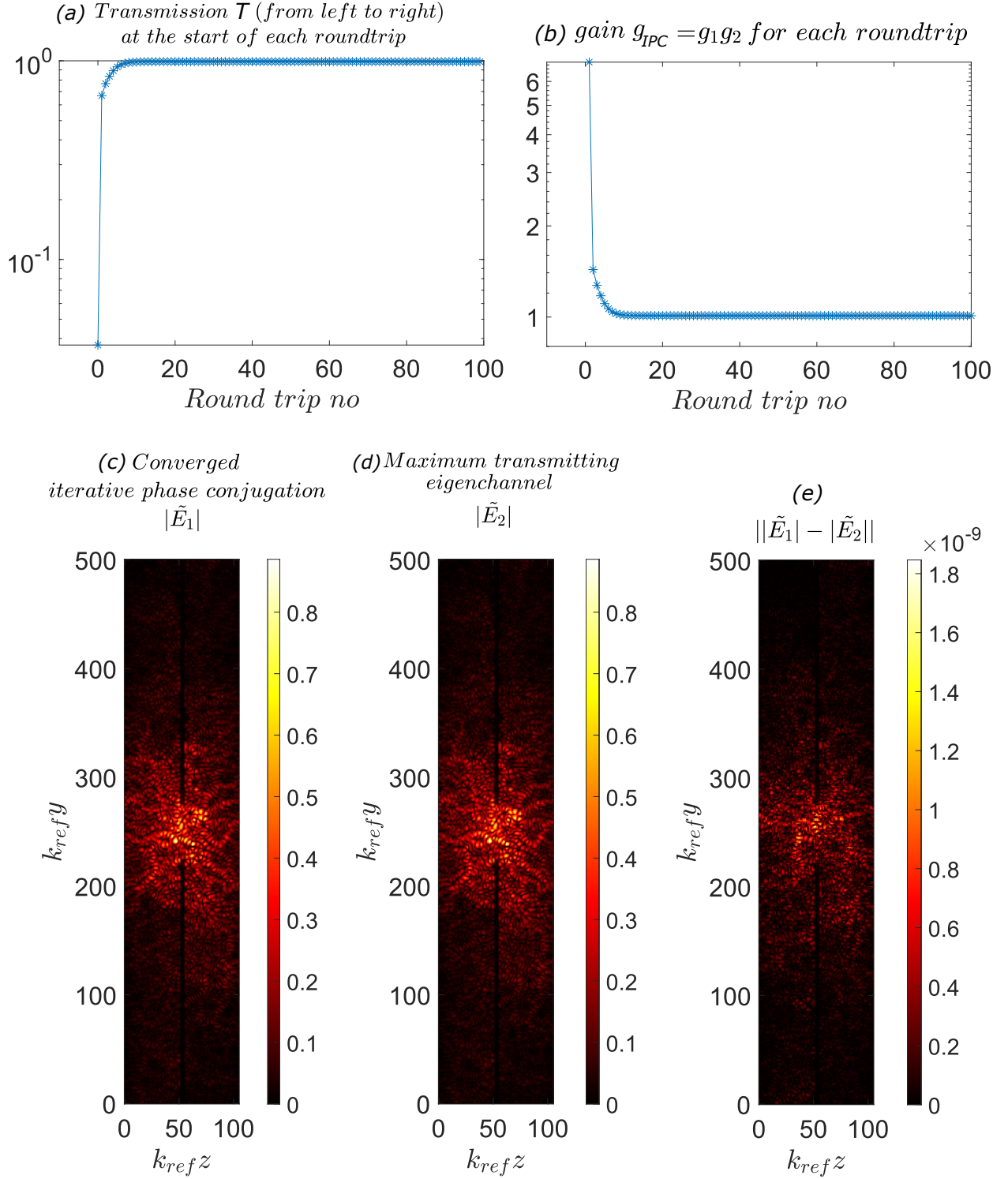


Figure 4.9: Iterative phase conjugation : Total transmission enhancement and gain vs round trip number. (a) Total transmission is plotted as a function of the number of round trips. The transmission increases (from the unshaped transmission value of 0.03707) and saturates to the same transmission value of 0.9899 corresponding to the maximally transmitting eigenchannel. (b) The gain profile is shown where comparatively larger values are needed towards the beginning (largest gain value being 6.9469). Upon the progress of the iterative phase conjugation process, the gain saturates to a comparatively lower value of 1.0102. (c) The magnitude of the converged iterative phase conjugation profile as demonstrated in Figure 4.8 (h), is reproduced again to compare against (d) the magnitude of the maximally transmitting eigenchannel, demonstrated in (a). (e) The magnitude of the difference between the magnitudes of the converged profile due to the iterative phase conjugation and the maximally transmitting eigenchannel is shown.

Until now, an aperture was used to observe about the increase of the wave transmission through a constriction inside a disorder, with wavefront shaping involving eigenchannels and iterative phase conjugation. For practical applications, the effect of the aperture is replaced by having a space-time modulated region surrounded by disordered region to undergo the iterative phase conjugation operation. Such an *STM* region acts as a tagged region surrounded by disorder through which the enhancement of total transmission is attempted through the iterative phase conjugation. Such a method has the potential¹⁰ to be used for tomographic applications inside diffusive scattering media. The numerical scheme implemented for the iterative phase conjugation process through a *STM* region is explained in the following section.

4.4 Focussing contrast in the Iterative phase conjugation through a Raman-Nath *STM* region in time domain

The *FDTD* method presented in Chapter 3, which involves an *STM* region and phase conjugation, is used in this section. The steps taken for the iterative phase conjugation scheme involving the *STM* modulation is summarised in the following steps. The *STM* region is switched on all the time during the iterative phase conjugation process.

Steps taken for the iterative phase conjugation through a *STM* region

1. Perform a forward propagation from the left to the right side of the disorder at the source temporal frequency of $\omega_{n=0}$. The multiply scattered light propagates through the *STM* region to generate harmonic wavefronts.
2. Perform the phase sensitive detection on the right side, of the $n = +1$ harmonic wavefront (up-converted wavefront in temporal frequency) at the temporal frequency $\omega_{n=+1} = \omega_0 + \omega_{mod}$, where ω_{mod} is the temporal modulation frequency of the *STM* region as explained in Chapter 3.
3. The detected wavefront at $\omega_{n=+1}$ is phase conjugated from the right side at the same temporal frequency $\omega_{n=+1}$ with a gain. Such a phase conjugate wave from the right, interacts with the *STM* region and get up-converted and down-converted in temporal frequency. But, only the down-converted wavefront at the $\omega_{n=0}$ by the *STM* region is detected on the left side in the next step.
4. Such a down-converted wavefront $\omega_{n=0}$, emerging only from the *STM* region and transmitted to the left side of the slab, undergoes phase sensitive detection on the left side at the temporal frequency $\omega_{n=0}$. Such a wavefront is phase conjugated once again with a gain at $\omega_{n=0}$ and set as an incident wave on the left side, completing one round trip.
5. Several such round trips are repeated phase conjugating the up-converted wavefront ($\omega_{n=1}$) from the right side and the down-converted wavefront ($\omega_{n=0}$) from the left. The key elements of the above given steps are shown in the Figure 4.10.

10: The advantage is that one could overcome multiple scattering to create a focus inside a disordered region. The limiting factors are the following. (1) The convergence of the iterative phase conjugation is competing against the decorrelation in tissue like media in practical scenarios. (2) The generation of a collection of foci by moving the *STM* region to different locations could be a time consuming serial process.

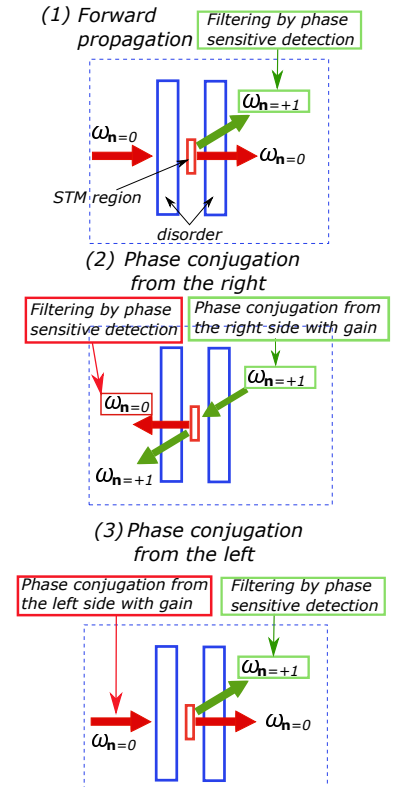


Figure 4.10: Main steps involved with the iterative phase conjugation through a space-time modulated region surrounded by disorder are shown. The steps are repeated for the iterative phase conjugation process.

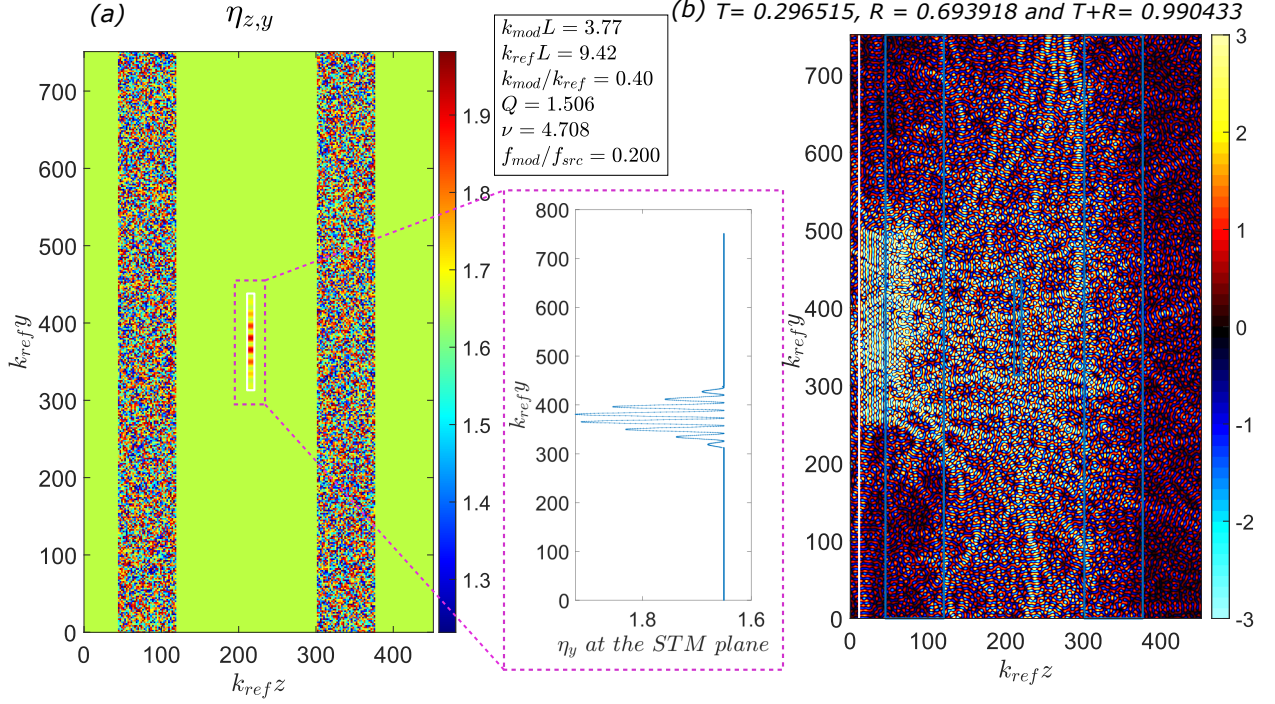


Figure 4.11: Geometry of the STM modulation in presence of disorder for the iterative phase conjugation process and the associated forward propagation (the first propagation from the left to right) are shown. (a) The refractive index associated with the computational domain is shown, where a Gaussian spatial modulation acting along the Y axis. The Gaussian modulation is set to travel from the bottom to the top, along the direction of +Y axis. **(b)** The forward propagation from the left side of the disorder when the STM region is switched-on, is plotted. The transmission and the reflection values given, are only for the combination of the slab disorders when the STM region is switched off. For the definition of the parameters such as Q , ν , etc., refer Chapter 3.

The effect of the disorder geometry and scattering properties on the iterative phase conjugation is studied by discussing it separately in two different subsections. First subsection uses a disorder geometry similar to that of the case given in Chapter 3, where the STM region is sandwiched between two disordered slabs, which is the configuration¹¹ that is usually seen in the experiments. The goal of the first subsection is to discuss the iterative phase conjugation process step-by-step for a given single realisation of the disorder. Such a given realisation of the disorder in the first subsection has the transmission properties similar that a disorder that lies in the diffusion-to-ballistic transition transport regime. Hence, some of the focussing trends that can be compared against experiments are discussed in the first subsection. The second subsection uses an extended single slab disorder instead of the sandwiched two-slab configuration. Four such different disordered slabs (with different transmission properties) are used to study the role played by multiple scattering on the focussing contrast, after 10 round-trips of iterative phase conjugation. For both the subsections, unlike that of Chapter 3, there is a Gaussian spatial modulation along the Y direction on the STM region as shown in Figure 4.11(a), providing a peak value of STM modulation at the center. In addition to that the STM region always switched on during the iterative phase conjugation process.

11: Such a disorder configuration, where the STM region is placed between two scattering media, is experimentally relevant because it gives a disorder-less region acting as a window to observe the focussing occurring between the two slabs.

4.4.1 Iterative phase conjugation method for the STM region placed between two disordered slabs

The forward propagation is shown in Figure 4.11(b).

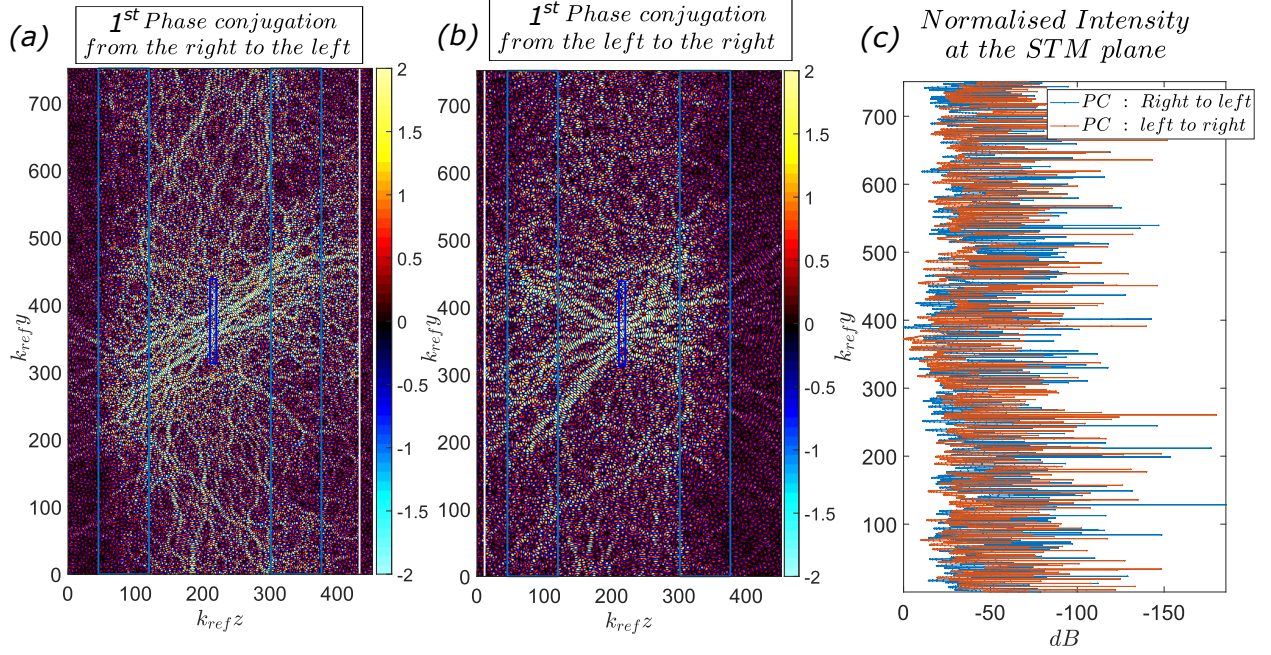


Figure 4.12: The first phase conjugation from the right side and the subsequent phase conjugation from the left side, with a STM modulated region surrounded by disorder, is shown. (a) Phase conjugation of the up-converted wavefront from the right side at $\omega_{n=+1}$ is shown. (b) Phase conjugation of the down-converted wavefront from the left at $\omega_{n=0}$ is plotted. (c) Intensity at the STM plane normalised with respect to the peak value, is plotted for both the cases. Also, both the field plots have clipped colour map limits, to make the focussing transport paths and the associated background region visible with sufficient contrast.

The first phase conjugation from the right side and the subsequent phase conjugation from the left side are shown in the Figure 4.12. Upon phase conjugation of the up-converted wavefront (at $\omega_{n=+1}$) from the right side with a gain, the wavefront retraces the direction of the up-converted wavefront (as shown in Figure 4.12(a)), which originally emerged from the STM region. A portion of such a phase conjugated wave propagating its way back to the STM region, gets down-converted and emerges onto the left side of the disorder, as indicated in the Figure 4.10(2). Such a wave gets phase conjugated from the left with a gain as shown in Figure 4.12(b), to interact with the STM region again, this time getting up-converted to the right side.

Upon the progress of round trips where the up-converted wavefront is phase conjugated from the right and the down-converted wavefront phase conjugated from the left, the focus becomes tighter along the transverse dimension, as shown in Figure 4.13. The focus becomes even narrower than the transverse length of the Gaussian modulated STM region. Such a phenomena was experimentally demonstrated by [4, 29] involving iterative phase conjugation and acousto-optic eigenchannels respectively. In the conventional acousto-optic imaging without any wavefront shaping involved, the resolution is limited to the diffraction limit of the acoustic wave (corresponding to the entire STM region in this chapter). In presence of wavefront shaping, especially with iterative phase conjugation or eigenchannels, such a conventional acoustic diffraction limit can be broken for the acousto-optic imaging as demonstrated in the Figure 4.14. It needs to be emphasised that the results shown in Figure 4.13 and Figure 4.14 are obtained for the two-slab geometry (given in Figure 4.11(a)) with a combined net transmission of 0.2965, where is the STM region was placed in the disorder-less region between the slabs. A

[29]: Si et al. (2012), 'Breaking the spatial resolution barrier via iterative sound-light interaction in deep tissue microscopy'

[4]: Katz et al. (2019), 'Controlling light in complex media beyond the acoustic diffraction-limit using the acousto-optic transmission matrix'

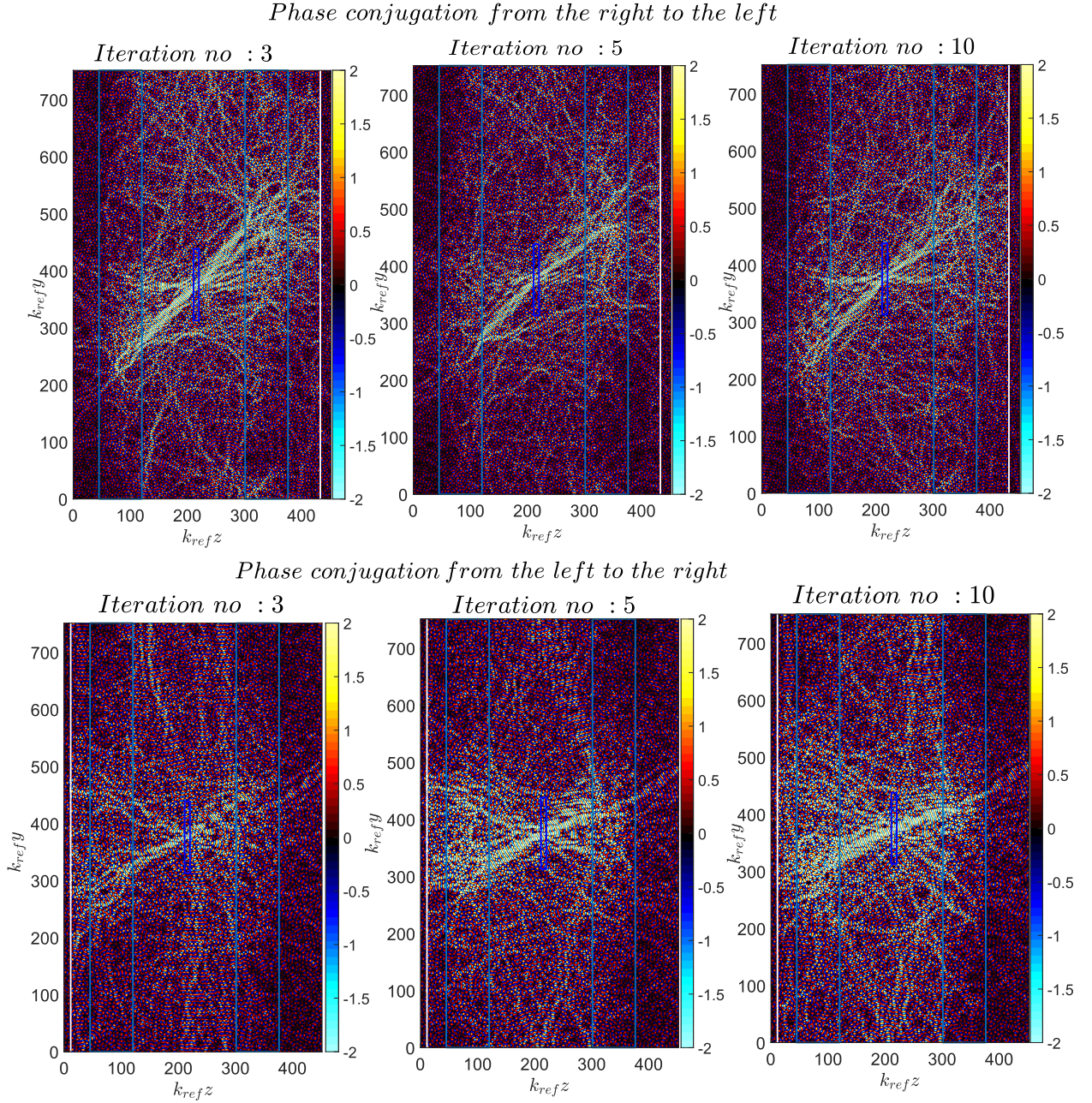


Figure 4.13: Demonstration of the field profile after several round trips of the iterative phase conjugation through an STM region. It can be seen from the plots that using the iterative phase conjugation method, the transverse size of focus formed is smaller than the STM region. As STM is a generalisation to the acousto-optic phenomena, this plot numerically demonstrates the idea that using iterative phase conjugation, the acoustic diffraction limit in the conventional acousto-optic imaging can be beaten. This is in agreement with the experimental observations given in Katz et al[4] who used acousto-optic eigenchannels for focussing the maximally transmitted eigenchannel and the Ke Si et al[29] who used iterative phase conjugation. Also, all the field plots have clipped colour map limits, to make the focussing transport paths and the associated background visible with sufficient contrast.

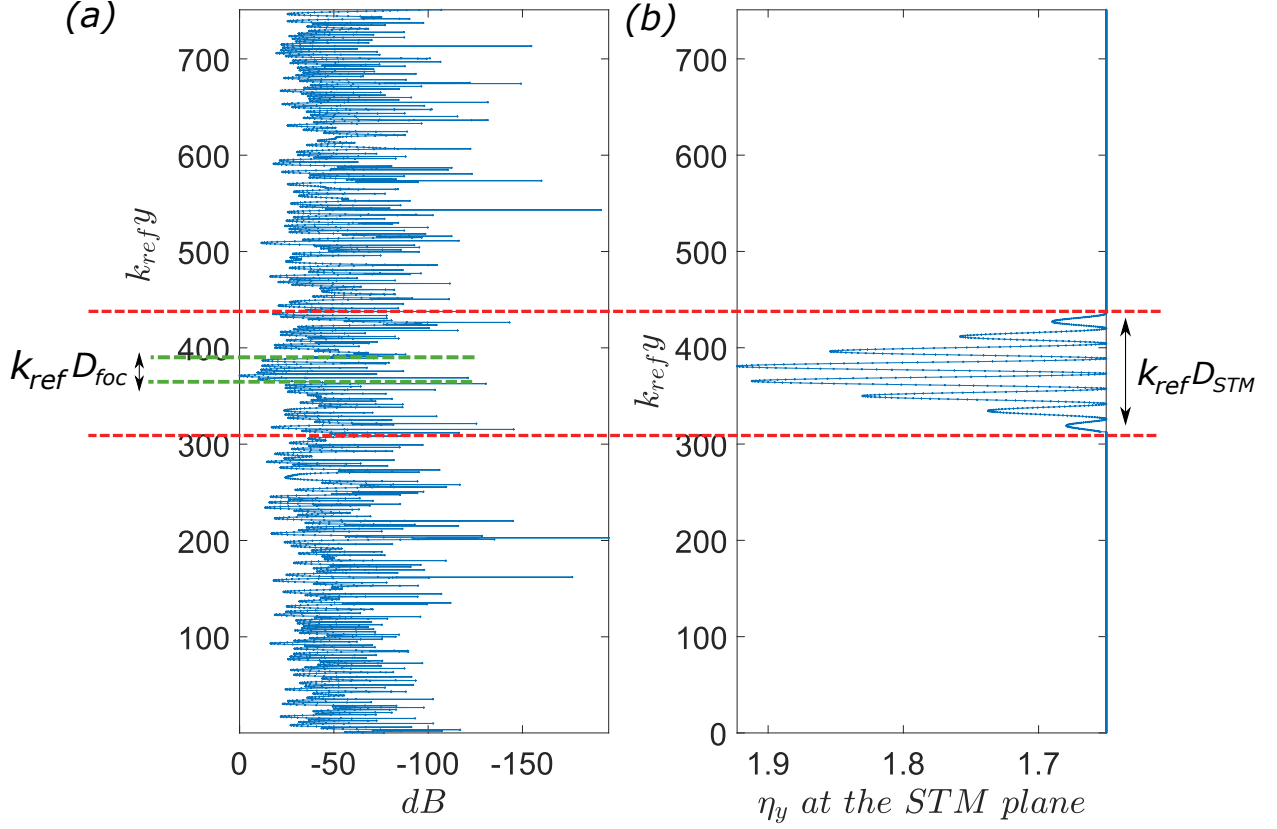


Figure 4.14: Comparison between the normalised focussing intensity at the STM y plane, due to the 10^{th} iterative phase conjugation with that of the STM refractive index profile, is shown. (a) The intensity of the focussing due to the phase conjugate wave from the right during the 10^{th} iteration is shown. The intensity is normalised with respect to the peak intensity. $k_{ref} D_{foc} = 22.806$ corresponds to the -24 dB point on both sides of the peak focus. (b) The transverse size of the STM modulation is shown where $k_{ref} D_{STM} = 126.166$. Therefore $D_{STM}/D_{foc} = 5.53214$.

disorder with such a transmission could be categorised as being in the diffusion-to-ballistic transition transport regime. This would naturally lead to the question of how a single extended disordered slab with an STM region embedded inside behaves under iterative phase conjugation and how the degree of multiple scattering plays a role in the focussing. Such a topic is discussed in the following subsection.

4.4.2 Iterative phase conjugation method for the STM region embedded inside a single extended disorder : The effect of multiple scattering

In this subsection, instead of the two slab disordered geometry taken before, a single extended slab disorder is considered such that the STM modulation is added on the top of the disorder refractive index, inside the slab. The STM parameters here are the same as taken before for the two slab geometry. Four such separate realisations of disorders are taken with increasing degree of scattering. In order to associate various transport regimes of these disorders, they shall be named as more-ballistic, less-ballistic, ballistic-to-diffusive transition and diffusive slab disorders with decreasing total transmission in that order. Total transmissions of these slabs during the forward propagation (without any STM modulation) are given in Figure 4.15. Iterative phase conjugation is performed on

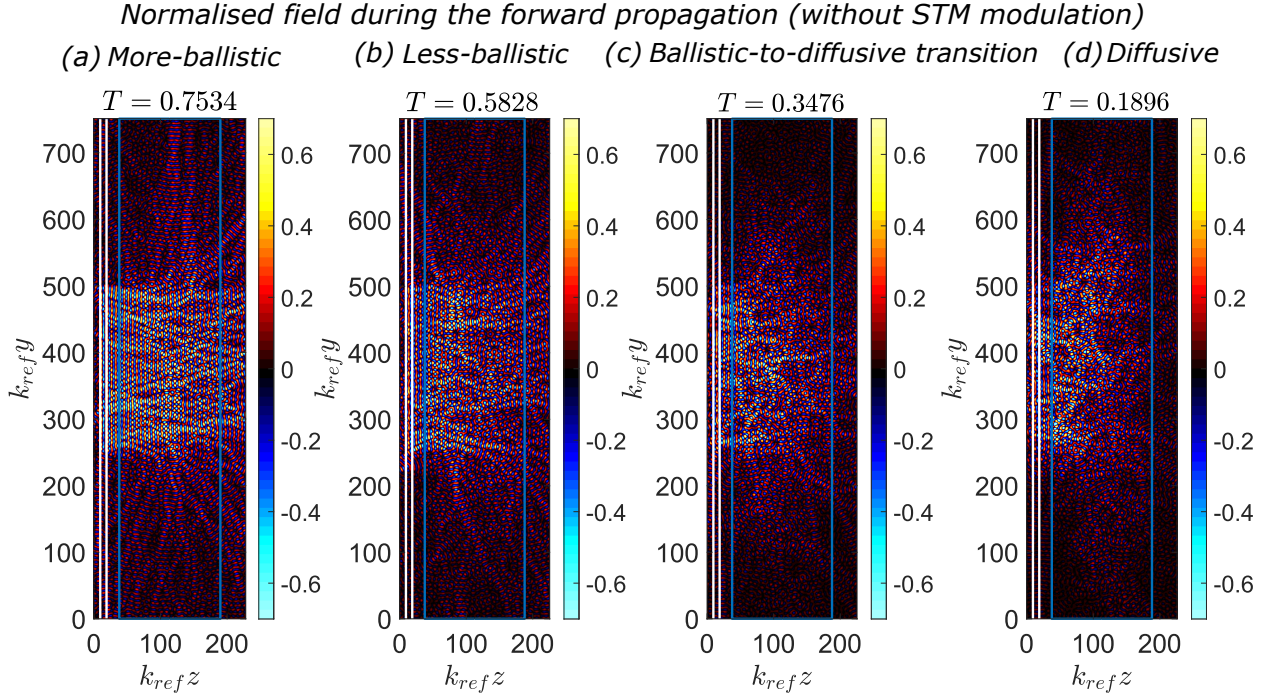


Figure 4.15: Plotting the forward propagation (without any STM) in four different disorder realisations, with decreasing total transmission, used later for the iterative phase conjugation with the STM modulation. The categories of the associated transport regimes and the total transmissions, T , are given for (a) the more-ballistic (b) the less-ballistic (c) ballistic-to-diffusion transition and (d) diffusive media. The individual field plots are normalised with respect to their peak field value. Iterative phase conjugation is performed on these disorders incorporating STM modulation and the field profiles in the 10th round trip are shown in Figure 4.16.

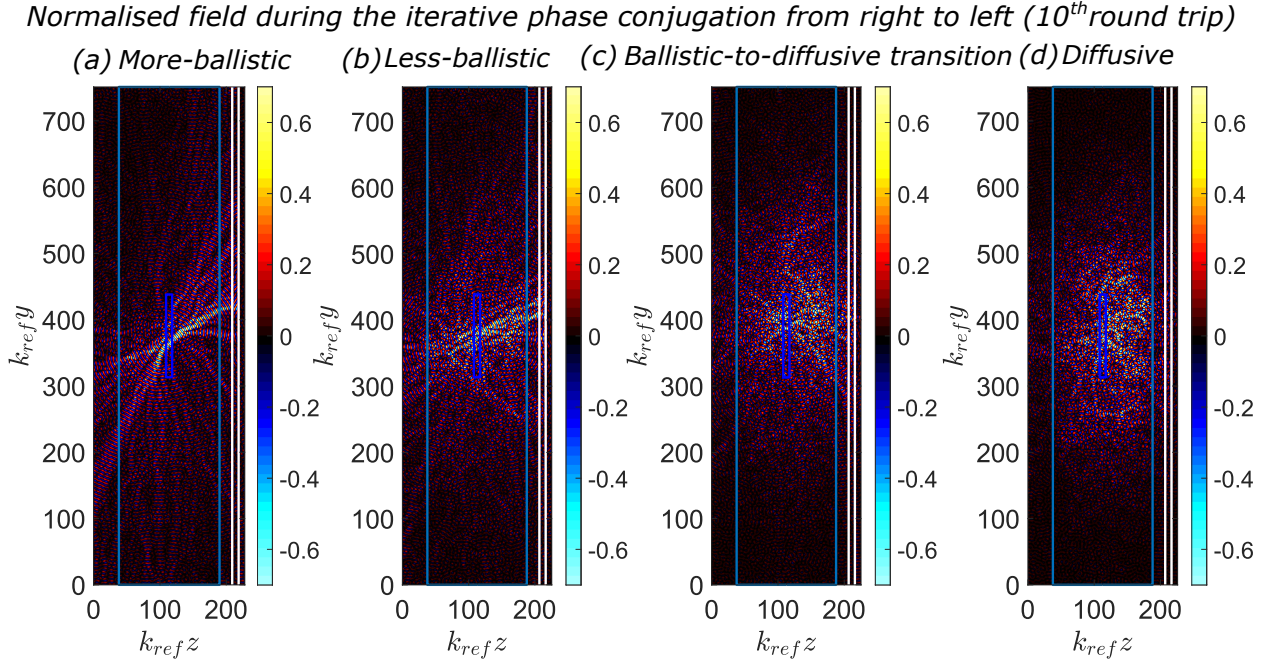


Figure 4.16: Plotting the field profile of the phase conjugation from right to left, during the 10th round trip of the iterative phase conjugation procedure, incorporating the STM modulation (enclosed in the blue rectangular region placed in the center of the slab), for the various transport regimes. The phase conjugation procedure starts with the incident beam profile shown in Figure 4.15 for the corresponding disorders. The individual phase conjugated field plots (in the 10th round trip) are normalised with their corresponding individual peak field value to estimate the contrast of the fields for (a) the more-ballistic (b) the less-ballistic (c) ballistic to diffusive transition and (d) diffusive media. The corresponding focussing intensity profiles at the STM region along the entire Y region, (with an averaging done along the Z region lying inside the STM), are plotted in Figure 4.17.

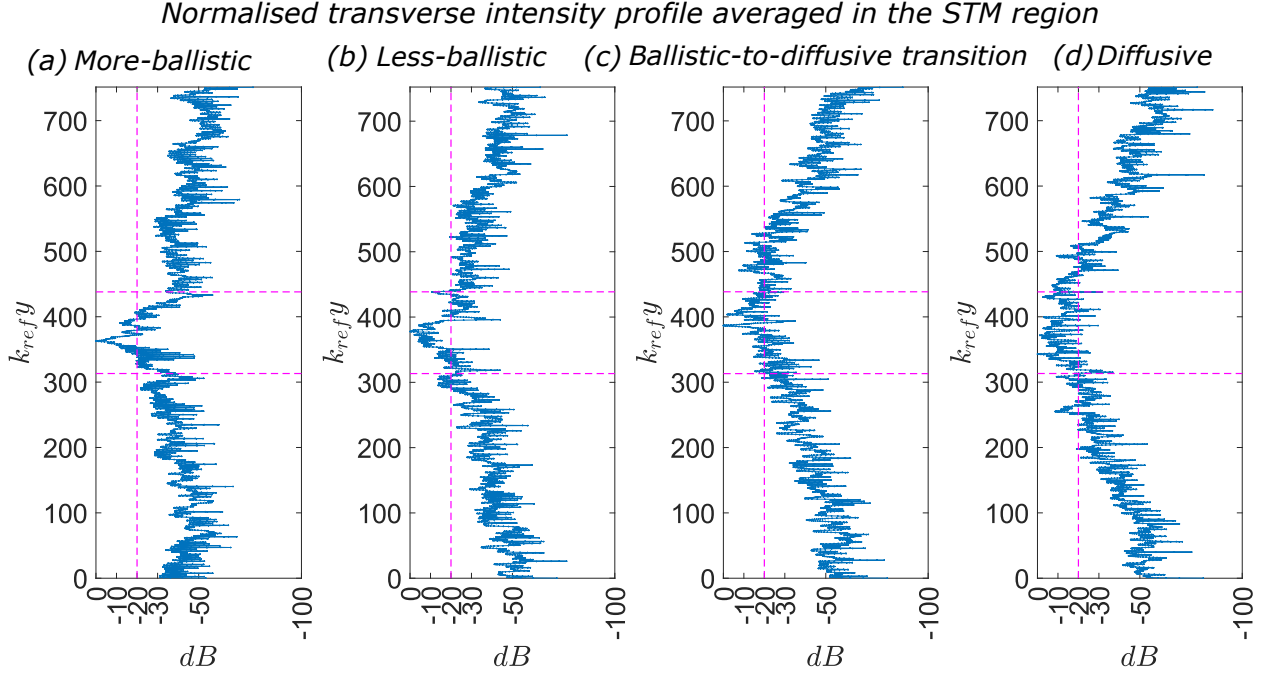


Figure 4.17: Plotting the normalised intensity at the *STM* region along Y , after averaging the intensity along the *STM* Z region, for the various iterative phase conjugation scenarios given in Figure 4.16. The averaged intensities are normalised with respect to the corresponding individual peak values of the averaged intensities for each of the samples, namely (a) more-ballistic (b) less-ballistic (c) ballistic-to-diffusion transition and (d) diffusive media. Normalisation with respect to the peak is to plot the contrast of the focus with respect to the background. Averaging of intensities is performed along the Z direction just for the z values lying inside the *STM* region's z boundaries, to average-out the intensity fluctuations in order to have better representation for comparison. The -20 dB intensity level is marked vertically as a dashed line. Similarly, the extent of the *STM* region along Y is marked using two horizontal dashed lines.

all four slabs following the same method as discussed before towards the beginning of Section 4.4. The peak-normalised field profiles inside the slabs due to the phase conjugation from the right to the left side of the slabs, in the 10^{th} round-trip of the iterative phase conjugation procedure, are plotted in Figure 4.16. The intensities inside the disorder at the *STM* region along Y , averaged along Z just in the *STM* region and normalised to the peak value, are given in Figure 4.17 for comparing the peak-to-background contrast for the four different kinds of disorders.

Such a study is done to visualise the effect of multiple scattering in the focussing operation via iterative phase conjugation. Observing the boxed region in Figure 4.17 around the focus (intersected by the three dashed lines and the Y axis), it can be observed that the focussing contrast reduces due to the increase in the degree of multiple scattering around the *STM* region. The reason for such a reduction in the contrast may be attributed to the physics of the problem being the effect of multiple scattering paths crossing each other, spread in-and-around the *STM* region in the extended slab, which the phase conjugate wave try to retrace as in time-reversal. At this point it is good to emphasise that in the sandwich geometry considered before in Figure 4.13, the *STM* region existed in the scattering-free region held between two scattering slabs, preventing the buildup of dense multiply-scattered paths within the *STM* region. In such a geometry, the two scattering slabs played the role of acting like large aperture scattering lens trying to focus onto an optically clear region tagged in between through *STM* modulation. A different possible reason for the reduction of contrast, this time due to the purely numerical method of *FDTD* time stepping and lock-in detection,

could be the numerical discretisation errors associated with the detection of the comparatively weaker *STM* modulated signal compared to the stronger unmodulated light. Further investigation in the future is needed to cross-verify whether there exist a fundamental limit based on the physics of the problem (independent of the numerical method used) for the contrast attained with respect to the degree of multiple scattering.

On a positive note, it can also be observed from Figure 4.16 and Figure 4.17 that with increasing degree of multiple scattering for iterative phase conjugation, there is increased confinement of light along the transverse dimension (along Y) inside the slab region (as the background of contrast decreases on the Y edges of the slab medium away from the *STM* region, with increased multiple scattering). Hence, even though the contrast decreases around the *STM* region for the diffusive disorder, the phase conjugate wave after several rounds of iterative phase conjugation, still remains confined inside the multiply scattering diffusive disorder along the transverse dimension. It also needs to be emphasised that in this thesis, the outgoing modulated waves are fully phase conjugated from both sides without any loss associated with the wave collection aperture, still giving the transverse confinement of waves inside the disorder. Therefore, even though the loss of contrast due to increased multiple scattering during iterative phase conjugation could be considered as a negative result, the transverse confinement of light in diffusive samples seems to be a positive result.

4.5 Conclusion

In the first half of the chapter, the equivalence between the iterative phase conjugation and the maximally transmitting eigenchannel, is numerically validated using the frequency domain modelling involving the S matrix of a disordered constriction. Here, the term “equivalence” refers to the observation that the wave intensity and the transmission profile obtained by performing iterative phase conjugation with a gain factor, converges to that of the case when the maximally transmitted eigenchannel is excited for the same disorder geometry. Therefore, in the context of experiments, instead of exciting the maximally transmitted eigenchannel (which requires the experimental measurement of the transmission matrix), one could perform iterative phase conjugation with a gain factor (which doesn’t require the experimental measurement of the transmission matrix) to obtain the same intensity and transmission profile obtained in the case of the maximally transmitted eigenchannel.

To numerically demonstrate such an equivalence between the iterative phase conjugation through an *STM* region and the corresponding maximally transmitting eigenchannel, access to the transmission matrix involving the *STM* region is necessary. Such a task of modelling the frequency domain transmission matrix incorporating a *STM* was challenging and it is yet to appear in the literature. Modelling the *STM* transmission matrix in the time domain was computationally tedious due to the large number of individual *FDTD* runs needed for many incident modes, achieving steady-state. Therefore, as the modelling of the *STM* transmission matrix was challenging, the modelling of iterative phase conjugation through an *STM* region was implemented in the time domain.

By extrapolating the same logic which was demonstrated in the first half of the chapter, the iterative phase conjugation profile through an *STM* region could be equivalent to the maximum transmitting eigenchannel through the *STM* region.

It is demonstrated using the modelling that the iterative phase conjugation method has the capacity to beat the acoustic diffraction limit in the conventional acousto-optic imaging, agreeing with the published experimental works. Also, the role played by multiple scattering on the focussing contrast inside an extended disorder, tagged by the *STM* modulation, is studied.

The main contribution of this thesis is the analytical and the numerical implementation of various wave transport modelling frameworks in the frequency domain and the time domain. This is for complementing the experimental works to be done in the future. The developed coding framework is intended to be published as open source packages with the GNU general public license. The contribution of chapter 1 is about the numerical estimation of the generalised S matrix using the generalisation of the conventional Fisher-Lee relations. An iterative method to evaluate the Green's function is also presented to save the memory during the perturbation process. The cascading of generalised S matrices in the frequency domain would be particularly advantageous in generating ensembles of disorders, which would otherwise be difficult in the time domain. The transmission matrices contained in the S matrix could be used to estimate the eigenchannels and also perform iterative phase conjugation from both sides of the disorder.

In chapter 2, the contribution is regarding the investigation on the role played by the spatial correlation of the disorder on various transport properties. Such a study is done with the help of the S matrices defined in chapter 1. The disorder spatial correlation can be varied to tailor the transport properties such as the scattering mean free path, the transport mean-free path and the anisotropy. Such a study on the effect of spatial correlation is particularly relevant in the case of biological tissues where there is always a finite spatial correlation length involved. The two parameter transmission scaling law is also presented which demonstrates the scalability of total transmission for a collection of disorders with different spatial correlation lengths. Therefore, the chapter dealt mostly with the statistical characterisation of the scattering properties of the disorder and the comparison between wave transport and diffusion theories.

Chapter 3 presents the formulation of the time domain methods where two time dependent phenomena are introduced. It includes the space-time modulation (STM) to be used as a guide-star for wavefront shaping and the Brownian decorrelation of the shaped wavefronts. The main contribution regarding the space-time modulation is the formulation of the wavefront shaping problem within the context of STM and performing the iterative phase conjugation. Such a study would be relevant for those wavefront shaping scenarios where a guide-star is used to focus inside the disordered region. For modelling the effect of defocussing due to Brownian motion, the Langevin $FDTD$ method was implemented, which is the next contribution provided in the chapter. Such a study combines the elements of non-equilibrium statistical mechanics with that of wavefront shaping.

The main contribution of chapter 4 are the following. The first is the modelling of the equivalence between the iterative phase conjugation process and the maximally transmitting eigenchannel through a disordered constriction. The second would be the simulation of breaking the acoustic diffraction limit in the context of conventional acousto-optic imaging, using iterative phase conjugation through a STM region. Such a study demonstrates the potential of using the acousto-optic phenomena for overcoming the multiple scattering of light in tissue like random media for focussing inside.

This thesis aimed to give a pedagogic analysis involving a collection of wavefront shaping modelling scenarios. If these scenarios are implemented experimentally for macroscopic biological media, that could be considered as novel techniques for pushing the research beyond the conventional diffuse optics involving just the incoherent transport of light. There are several experimental challenges involved, ranging from fast holographic phase measurement and the associated wavefront shaping technique, to addressing the problem of decorrelation in random media. Hopefully, the experimental challenges would be overcome in the near future to start applying these concepts for practical applications in the field of biophotonics.

In this section, some of my personal reflective thoughts regarding the research done is presented.

The main goal of my Ph.D studies was to develop various modelling frameworks to investigate a collection of wavefront shaping applications that could be relevant for biophotonics applications. Towards the beginning of the PhD program, the topics given in the thesis were set as the target to be achieved. The pondering question in the beginning was, for the given collection of topics, what would the best course of action be such that the goal could be achieved within the duration of the PhD program. The concepts had to be learned and implemented from the scratch by me. The first 6-8 months were devoted to study the feasibility of choosing various models to begin with, so that the goals could be achieved eventually within the research duration. The scope for using the Monte Carlo random walker for the transport applications involving wavefront shaping was initially investigated and quickly dropped due to the realisation that it won't be sufficient. The Monte Carlo random walker which derives its existence from the incoherent transport theory, lacked the idea of source coherence for interference and the time-reversal symmetry, which were needed in the context of wavefront shaping in non-absorbing media. This naturally lead to studying about the wave transport in random media for various wavefront shaping scenarios and also its relationship with diffusion theory.

The next question to be addressed initially was whether to model the wave transport problem in 3D with large number of scatterers. Considering the topics presented in the thesis, such a task of implementing those topics as a 3D problem involving large number of scatterers, was challenging due to the large memory requirement, the computational power required and the available time for the PhD programme. The task of large scale 3D wave scattering simulation involving millions of scatterers is a PhD research by itself and was not within the scope of my studies. Instead, the 2D transport problem was studied and got it related to the scattering matrix. The statistical, transport and conservation properties of these scattering matrices are the same, irrespective of the problem being 3D or 2D in the diffusion regime. The transmission scaling law also helped, as one could address various transport problems in terms of L/l^* as a dimensionless parameter. Therefore, most of the transport theory results presented in the thesis is expected to hold true, even with the larger 3D modelling. Thus, taking the decision of using the 2D models helped to hold onto the original goal for completing it.

Another consideration in the beginning for choosing a particular formalism for the given problem was regarding the trade-off between memory efficiency and flexibility. The question was whether one should prioritise flexibility-of-use over the memory efficiency for solving the scattering problem. As an example, the Green's function method presented in the thesis is not very memory efficient (due to the need for storing and perturbing the Green's function themselves) for solving the scattering problem in general, but it is flexible in several ways. First of all, there exist the analytical perturbation theory involving Green's function which could be used as a guidance for the code development to test the correctness of the modelling implemented. Secondly, the perturbation theory is an elegant way of solving the scattering problem from the physics point of view (although not so memory efficient). This is because, all the mathematical properties associated with the basis wave modes, the associated wave flux and the Green's function are well defined even before the perturbation process starts, giving us the ability to obtain exact results without much numerical error involved. Similarly, for those topics where the frequency domain techniques were tough to implement, the finite difference time domain method (FDTD) was chosen. The FDTD method is very flexible, where the required bells and whistles can be implemented as we progress through the coding. Such a FDTD method is easy to use and intuitive to understand, but couldn't be compared against the analytical elegance and tractability of the frequency domain perturbation theory.

Another challenge faced was to review the mesoscopic wave transport theory, which was mostly studied around the quantum theory of coherent wave transport. Coming from an engineering background, made my

learning curve steeper than what was generally felt by a student from the physics background. This is also a reason why classical theory of wave transport is presented in the thesis, without using much notations and formalisms from the quantum transport. Nevertheless, an attempt was made to make the thesis a physics thesis rather than an engineering thesis, as I was affiliated to the physics department. Such a point was made clear by the graduate supervision committee from the early stage that the committee expects a thesis discussing the physics of the problem and not on the engineering or the biomedical applications.

For developing the codes, mostly Matlab and Mathematica were used. This was mainly for the quicker prototyping of the numerical coding frameworks in Matlab, after deriving and verifying the analytical results with the help of Mathematica. Such a combination of using Mathematica and Matlab was felt essential in this line of work. The power of symbolic computation in Mathematica is particularly appreciated for the kind of work presented in the thesis. As hinted in the quote given towards the beginning of the thesis, personally I enjoyed doing the analytical part of the thesis more than the purely numerical part of it. As it is tough to address everything just analytically, compromises had to be made to use purely numerical modelling methods such as *FDTD*.

A considerable portion of my time for the PhD was consumed for testing the developed codes to ensure the validation of all sorts of conservation and symmetry principles involved. Availability of various conservation laws helped for the testing to ensure the correctness of the developed frameworks. Also, no free parameters are defined in this thesis. All the parameters defined can be analytically related back to a first principle method or expression. Lincoln's quote on sharpening his axe for the first 4 hours to cut a tree in 6 hours, is apt to be said here for taking one's time for testing these fundamental principles and ensuring not to use any free parameters. Spending hours and days for ensuring the correctness of the code, debugging for issues is the norm than getting everything right in the first instance itself.

The thesis is presented taking a conservative stand regarding the formalisms presented. Traditionally used formalisms and ideas are frequently revisited and used as a stepping stone to explore new ideas. Therefore, a certain degree of conformity was needed with the existing "old school" literature which helped being on track without getting lost in the research.

Looking back in hindsight after learning through the presented methods, one could always ask whether the models could have been made better. Instead of using the numerical grid in the frequency domain, one could implement cylindrical or spherical harmonic modes and the T matrix method for evaluating the scattering, especially involving resonant scatterers and periodic boundary conditions. The wavefront shaping through the *STM* region could have been implemented in the frequency domain, instead of the presented time domain method. Such a method could have naturally yielded a transmission matrix in the frequency domain involving a *STM* region. Instead of the scalar boundary integral formulation, the vector boundary integral version together with the Dyadic Green's function, could have been used to address the subject as a light transport problem. Incorporating losses in the medium (or losses in the collection of modes) could have been a possible extension of the studies for all the chapters. The aspects of controllability of the number of input modes could have been studied for the presented contents of the thesis. The memory effect associated with the focussing involving a *STM* region could be investigated. On an optimistic note, these aspects could be considered as future works, to improve upon the works presented in the thesis.

APPENDIX

Appendix

A.1 Definition of Fourier transform used

For time-frequency Fourier transform, the following convention is used

$$\mathcal{F}\{f(t)\} = F(\omega) = \int_{-\infty}^{+\infty} f(t)e^{-i\omega t} dt \quad (\text{A.1})$$

$$\mathcal{F}^{-1}\{F(\omega)\} = f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega)e^{i\omega t} d\omega \quad (\text{A.2})$$

where $\mathcal{F}$ denotes the Fourier operator and $\mathcal{F}^{-1}$ the inverse Fourier operator. Then, it follows that

$$\frac{d^k f(t)}{dt^k} = (i\omega)^k F(\omega) \quad (\text{A.3})$$

A.2 Scalar Helmholtz wave equation from Maxwell's equations in 2D

Source free Maxwell's equations[107] are given as

$$\nabla \times H(r, t) = \frac{\partial D(r, t)}{\partial t} \quad (\text{A.4})$$

$$\nabla \times E(r, t) = \frac{-\partial B(r, t)}{\partial t} \quad (\text{A.5})$$

$$\nabla \cdot D(r, t) = 0 \quad (\text{A.6})$$

$$\nabla \cdot B(r, t) = 0 \quad (\text{A.7})$$

where $E(r, t)$ is the electric field intensity, $D(r, t)$ the electric flux density, $H(r, t)$ the magnetic field intensity and $B(r, t)$ the magnetic flux density. In addition to the Maxwell's equations, the following constitutive relations are needed for forming a wave equation from the curl equations.

$$D(r, t) = \epsilon(r, t) * E(r, t) \quad (\text{A.8})$$

$$B(r, t) = \mu(r, t) * H(r, t) \quad (\text{A.9})$$

where $\epsilon(r, t)$ is the dielectric permittivity, $\mu(r, t)$ the permeability and $*$ denotes convolution in time. $\epsilon(r, t) = \epsilon_0 \epsilon_r(r, t)$ where ϵ_0 is the free space permittivity and $\epsilon_r(r, t)$ the relative dielectric constant with respect to free space. It is assumed that the disordered medium is not varying magnetically in space and time. Such an assumption is usually valid in biological medium. Hence $\mu(r, t) = \mu_0 \mu_r$ where μ_0 is the free space permeability and μ_r the relative permeability constant usually taken as unity. Therefore the constitutive relation involving magnetic fields could be written as

$$B(r, t) = \mu_0 \mu_r H(r, t) \quad (\text{A.10})$$

Substituting the above given relation in the curl equation, equation A.5 gives

$$\nabla \times E(r, t) = -\mu_0 \mu_r \frac{\partial H(r, t)}{\partial t} \quad (\text{A.11})$$

which on Fourier transform with respect to time (refer to Section A.1 for the convention used) yields

$$\begin{aligned} \nabla \times \tilde{E}(r, \omega) &= -i\omega \mu_0 \mu_r \tilde{H}(r, \omega) \implies \\ \tilde{H}(r, \omega) &= \frac{\nabla \times \tilde{E}(r, \omega)}{-i\omega \mu_0 \mu_r} \end{aligned} \quad (\text{A.12})$$

Similarly, the magnetic field curl equation (equation A.4) can be Fourier transformed with respect to time to obtain

$$\nabla \times \tilde{H}(r, \omega) = i\omega \tilde{D}(r, \omega) \quad (\text{A.13})$$

As convolution transforms into products in Fourier transform domain, the electric field constitutive relation transforms into

$$\tilde{D}(r, \omega) = \tilde{\epsilon}(r, \omega) \tilde{E}(r, \omega)$$

Substituting the above given constitutive relation in the Fourier transformed magnetic curl equation (equation A.13),

$$\nabla \times \tilde{H}(r, \omega) = i\omega \epsilon_0 \tilde{\epsilon}_r(r, \omega) \tilde{E}(r, \omega) \quad (\text{A.14})$$

Substituting for $\tilde{H}(r, \omega)$ using Eq A.12

$$\nabla \times \nabla \times \left\{ \frac{\tilde{E}(r, \omega)}{-i\omega \mu_0 \mu_r} \right\} = i\omega \epsilon_0 \tilde{\epsilon}_r(r, \omega) \tilde{E}(r, \omega) \implies \quad (\text{A.15})$$

$$\nabla \times \nabla \times \tilde{E}(r, \omega) = \omega^2 \mu_0 \epsilon_0 \mu_r \tilde{\epsilon}_r(r, \omega) \tilde{E}(r, \omega) \quad (\text{A.16})$$

Define wave vector $k_0 = 2\pi/\lambda_0 = 2\pi f/c = \omega/c = \omega\sqrt{\epsilon_0 \mu_0}$ where f is the linear temporal frequency, λ_0 the wavelength and $c = 1/\sqrt{\mu_0 \epsilon_0}$ is the wave velocity.

$$\nabla \times \nabla \times \tilde{E}(r, \omega) = k_0^2 \mu_r \tilde{\epsilon}_r(r, \omega) \tilde{E}(r, \omega) \quad (\text{A.17})$$

Using the curl-of-a-curl vector identity on the *L.H.S* of the equation A.17, it could be written as

$$\begin{aligned} \nabla \times \nabla \times \tilde{E}(r, \omega) &= \nabla[\nabla \cdot \tilde{E}(r, \omega)] - \nabla^2 \tilde{E}(r, \omega) \\ &= k_0^2 \mu_r \epsilon_r(r, \omega) \tilde{E}(r, \omega) \end{aligned} \quad (\text{A.18})$$

Hence, the vector wave equation is given as

$$\nabla[\nabla \cdot \tilde{E}(r, \omega)] - \nabla^2 \tilde{E}(r, \omega) = k_0^2 \mu_r \epsilon_r(r, \omega) \tilde{E}(r, \omega) \quad (\text{A.19})$$

As the main theme of the thesis is the 2D wave transport phenomena in random media involving multiple scattering, the above given vector wave equation is simplified into a scalar wave equation in the following section. In addition to that, in experiments it is assumed that the polarisation of the outgoing wave would be sufficiently randomised by the random scattering. Hence the next section aims to simplify $\nabla[\nabla \cdot \tilde{E}(r, \omega)]$ in such a way that it helps to form a simpler scalar wave equation. For that, the following vector calculus identity involving a general vector field A and a non-zero scalar

field ϕ is used

$$\begin{aligned}\nabla \cdot (\phi A) &= \phi \nabla \cdot A + A \cdot \nabla \phi \implies \frac{1}{\phi} \nabla \cdot (\phi A) = \nabla \cdot A + \frac{1}{\phi} A \cdot \nabla \phi \implies \\ \frac{1}{\phi} \nabla \cdot (\phi A) - \frac{1}{\phi} A \cdot \nabla \phi &= \nabla \cdot A\end{aligned}\quad (\text{A.20})$$

Applying the above given vector identity to $\nabla \cdot \tilde{E}(r, \omega)$ where $\tilde{E}(r, \omega)$ is the vector field and $\tilde{\epsilon}_r(r, \omega)$ the non zero scalar field,

$$\frac{1}{\tilde{\epsilon}_r(r, \omega)} \nabla \cdot [\tilde{\epsilon}_r(r, \omega) \tilde{E}(r, \omega)] - \frac{1}{\epsilon_r(r, \omega)} \tilde{E}(r, \omega) \cdot \nabla \tilde{\epsilon}_r(r, \omega) = \nabla \cdot \tilde{E}(r, \omega) \quad (\text{A.21})$$

By the divergence theorem of Maxwell's equation (equation A.6),

$$\nabla \cdot \tilde{D}(r, \omega) = \nabla \cdot [\tilde{\epsilon}_r(r, \omega) \tilde{E}(r, \omega)] = 0 \quad (\text{A.22})$$

Substituting the result from divergence theorem back in Eq A.21

$$-\frac{1}{\tilde{\epsilon}_r(r, \omega)} \tilde{E}(r, \omega) \cdot \nabla \tilde{\epsilon}_r(r, \omega) = \nabla \cdot \tilde{E}(r, \omega) \quad (\text{A.23})$$

This implies that for a non-zero $\tilde{E}$ field, $\nabla \cdot \tilde{E}(r, \omega)$ is zero under either of the two following conditions [108]

- $\nabla \tilde{\epsilon}_r(r, \omega) = 0$, implying no scatterer variation (uniform medium)
- Or
- If $\tilde{E}(r, \omega)$ has a polarisation such that $E(r, \omega) \perp \nabla \epsilon_r(r, \omega)$, then $\nabla \cdot \tilde{E}(r, \omega) = 0$. This is particularly valid in the 2D scattering scenario, implying that if $E(r, \omega)$ is perpendicular to the gradient of $\epsilon_r(r, \omega)$, $\nabla \cdot E(r, \omega) = 0$. In other words, if the $E(r, \omega)$ is polarised perpendicular to the direction of variation of the dielectric scattering variation, then $\nabla \cdot \tilde{E}(r, \omega) = 0$.

Substituting $\nabla \cdot \tilde{E}(r, \omega) = 0$ in the vector wave equation (equation A.19), it reduces to the scalar wave equation as given below for 2D scattering

$$\nabla^2 \tilde{E}(r, \omega) + k_0^2 \mu_r \tilde{\epsilon}_r(r, \omega) \tilde{E}(r, \omega) = 0 \implies [\nabla^2 + k_0^2 \mu_r \tilde{\epsilon}_r(r, \omega)] \tilde{E}(r, \omega) = 0$$

Such a scalar wave equation called as the Helmholtz wave equation, is used throughout this thesis for estimating the light transport properties in random media.

A.3 Analytical $G_0(r, r_0)$ for the wave equation with transverse mirror boundaries

As the harmonic time dependence is given as $e^{-i\omega t}$ with the negative sign in the argument of the exponential, it causes $e^{i(k_z z - \omega t)}$ to be a wave travelling along the +z direction when time progresses. First, consider the 1D problem along z axis and after that, it would be generalised to the 2D scenario.

A.3.1 1D analytical Green's function for the wave equation along z axis

Consider the 1D propagation of a wave originating from a Dirac delta source placed at z_0 . The 1D form of the scalar Helmholtz equation (without disorder) is given as

$$\left[\frac{d^2}{dz^2} + (k_z^{ref})^2 \right] G_0^z(z, z_0) = \delta(z - z_0) \quad (\text{A.24})$$

with outgoing boundary condition along z axis. In words, the above equation can be described as a second order differential operator acting on $G_0^z(r, r_0)$ yielding a Dirac delta on the R.H.S. It implies that the first order derivative should have a jump discontinuity (refer chapter 3.3 of [42]) and the expression of $G_0^z(z, z_0)$ should be continuous at z_0 . Integrating equation A.24 around the neighbourhood of z_0 ,

$$\begin{aligned} \lim_{\delta \rightarrow 0} \left[\int_{z_0-\delta}^{z_0+\delta} \frac{d^2}{dz^2} G_0^z(z, z_0) dz + (k_z^{ref})^2 \int_{z_0-\delta}^{z_0+\delta} G_0^z(z, z_0) dz \right] &= \lim_{\delta \rightarrow 0} \int_{z_0-\delta}^{z_0+\delta} \delta(z - z_0) dz \implies \\ \lim_{\delta \rightarrow 0} \frac{d}{dz} G_0^z(z, z_0) \Big|_{z_0-\delta}^{z_0+\delta} + (k_z^{ref})^2 \times 0 &= 1 \quad \because G_0^z(z, z_0) \text{ is continuous at } z_0 \implies \\ \lim_{\delta \rightarrow 0} \left[\frac{d}{dz} G_0^z(z, z_0) \Big|_{z_0+\delta} - \frac{d}{dz} G_0^z(z, z_0) \Big|_{z_0-\delta} \right] &= 1 \end{aligned} \quad (\text{A.25})$$

This implies that there is a jump discontinuity for the first order derivative at $z = z_0$. Consider a test solution of the form given below which satisfies the 1D Helmholtz equation given in equation A.24

$$G_0^z(z, z_0) = \begin{cases} G_0^+(z, z_0) = c^+ e^{i[k_z^{ref}(z-z_0)]}, & \text{if } z \geq z_0 \\ G_0^-(z, z_0) = c^- e^{i[-k_z^{ref}(z-z_0)]}, & \text{if } z < z_0 \end{cases} \quad (\text{A.26})$$

Test solution should be continuous at $z = z_0$ therefore $G_0^+(z, z_0)|_{z=z_0} = G_0^-(z, z_0)|_{z=z_0}$ and it forces $c^+ = c^- = c$. Substituting the test solution into equation A.25

$$\begin{aligned} \lim_{\delta \rightarrow 0} [(ik_z^{ref})c^+ e^{i[k_z^{ref}(z-z_0)]} \Big|_{z=z_0+\delta} - (-ik_z^{ref})c^- e^{i[-k_z^{ref}(z-z_0)]} \Big|_{z=z_0-\delta}] &= 1 \implies \\ (ik_z^{ref})c^+ + (ik_z^{ref})c^- &= 1 \end{aligned} \quad (\text{A.27})$$

As $c^+ = c^- = c_0$, the above given equation is solved to obtain $c_0 = 1/(2ik_z^{ref})$. Therefore,

$$G_0^z(z, z_0) = \begin{cases} G_0^+(z, z_0) = \frac{1}{2ik_z^{ref}} e^{i[k_z^{ref}(z-z_0)]}, & \text{if } z \geq z_0 \\ G_0^-(z, z_0) = \frac{1}{2ik_z^{ref}} e^{i[-k_z^{ref}(z-z_0)]}, & \text{if } z < z_0 \end{cases} \quad (\text{A.28})$$

Using the modulus function, $G_0^z(z, z_0)$ could be written generally as

$$G_0^z(z, z_0) = \frac{1}{2ik_z^{ref}} e^{i|k_z^{ref}(z-z_0)|} \quad z \in \mathcal{R}^1 \quad (\text{A.29})$$

A.3.2 1D analytical eigenfunctions for the wave equation along y axis

Along the transverse dimension (y axis), the boundary condition is different (from that given in Section A.3.1) that it is not the outgoing boundary condition, but a reflection (also called as a zero/mirror/Dirichlet) boundary condition. Let $\chi(y)$ be an arbitrary wave along the y dimension

$$\left[\frac{d^2}{dy^2} + (k_y^{ref})^2 \right] \chi(y) = 0 \quad (\text{A.30})$$

with boundary conditions such that $\chi(y = 0) = 0$ and $\chi(y = W) = 0$ which are the zero(reflection) boundary conditions. The equation A.30 is a familiar equation in physics drawing its similarity to the "particle in a box" problem. Hence, the solution $\chi(y)$ could be expanded in terms of the eigenfunctions in the 1D cavity as the eigenfunctions form a complete 1D basis set in $(0, W)$. Let the m^{th} transverse eigenfunction be represented as

$$\chi_m(y) = \sqrt{\frac{2}{W}} \sin(k_y^{(m)} y), \quad (\text{A.31})$$

where $k_y^{(m)} = m\pi/W$ and $m = 1, 2, 3...etc$. These eigenfunctions satisfy equation A.30 individually as given below

$$\left[\frac{d^2}{dy^2} + (k_y^{(m)})^2\right]\chi_m(y) = 0 \quad (\text{A.32})$$

Next, the orthogonality and the completeness properties [39] of the basis set is given. As $\chi_m(y)$ is a real function,

Orthogonality property

$$\langle \chi_m(y) | \chi_n(y) \rangle = \int_0^W \chi_m(y)^* \chi_n(y) dy = \int_0^W \chi_m(y) \chi_n(y) dy = \delta_{kron}(m, n) \quad (\text{A.33})$$

where $\delta_{kron}(m, n)$ is the Kronecker delta function such that $\delta_{kron}(m, n) = 1$ only when $m = n$ and zero otherwise.

Completeness property : Any arbitrary function $f(y)$ in the domain spanned by the basis set can be expanded in terms of its basis elements.

$$f(y) = \sum_{m=1}^{\infty} c_m \chi_m(y) \quad (\text{A.34})$$

As an example, let $f(y) = \delta(y - y_0)$, then the coefficients of expansion

$$c_n = \int_0^W \chi_n(y) \delta(y - y_0) dy = \langle \chi_n(y) | \delta(y - y_0) \rangle = \chi_n(y_0) \quad (\because \text{sifting property of Dirac delta}) \quad (\text{A.35})$$

Therefore, $f(y) = \delta(y - y_0)$ can be expanded as

$$\delta(y - y_0) = \sum_{m=1}^{\infty} c_m \chi_m(y) = \sum_{m=1}^{\infty} \chi_m(y_0) \chi_m(y) \quad (\text{A.36})$$

A.3.3 2D analytical Green's function for the wave equation, $G_0(r, r_0)$ in uniform medium

Using the ideas developed in the previously given subsections, (Section A.3.1 and Section A.3.2), $G_0(r, r_0)$ in 2D is solved as given below. Consider the 2D scalar Helmholtz equation without disorder.

$$[\nabla^2 + k_{ref}^2]G_0(z, y, z_0, y_0) = \delta(z - z_0)\delta(y - y_0) \quad (\text{A.37})$$

Let $G_0(z, y, z_0, y_0)$ be expanded[39] as

$$G_0(z, y, z_0, y_0) = \sum_{m=1}^{\infty} \phi_m(z, z_0) \chi_m(y) \chi_m(y_0) \quad (\text{A.38})$$

Substituting the above given expansion in equation A.37,

$$[\nabla^2 + k_{ref}^2] \sum_{m=1}^{\infty} \phi_m(z, z_0) \chi_m(y) \chi_m(y_0) = \delta(z - z_0)\delta(y - y_0) \quad (\text{A.39})$$

Substituting the expansion of Dirac delta function given in equation A.36 into the previous equation,

$$[\nabla^2 + k_{ref}^2] \sum_{m=1}^{\infty} \phi_m(z, z_0) \chi_m(y) \chi_m(y_0) = \delta(z - z_0) \sum_{m=1}^{\infty} \chi_m(y_0) \chi_m(y) \quad (A.40)$$

Re-arranging the above equation as

$$\sum_{m=1}^{\infty} \chi_m(y_0) \left[\frac{d^2}{dz^2} + \frac{d^2}{dy^2} + k_{ref}^2 \right] \phi_m(z, z_0) \chi_m(y) = \sum_{m=1}^{\infty} \delta(z - z_0) \chi_m(y_0) \chi_m(y) \quad (A.41)$$

L.H.S of the above given equation is

$$\sum_{m=1}^{\infty} \chi_m(y_0) \left[\chi_m(y) \frac{d^2}{dz^2} \phi_m(z, z_0) + \phi_m(z, z_0) \frac{d^2}{dy^2} \chi_m(y) + k_{ref}^2 \phi_m(z, z_0) \chi_m(y) \right] \quad (A.42)$$

Using equation A.32 for m^{th} eigenfunction

$$\frac{d^2}{dy^2} \chi_m(y) = -(k_y^{(m)})^2 \chi_m(y) \quad (A.43)$$

Substituting eq. A.43 in eq.A.42, the L.H.S of eq.A.41 could be simplified as

$$\begin{aligned} L.H.S &= \sum_{m=1}^{\infty} \chi_m(y_0) \left[\chi_m(y) \frac{d^2}{dz^2} \phi_m(z, z_0) - \phi_m(z, z_0) (k_y^{(m)})^2 \chi_m(y) + k_{ref}^2 \phi_m(z, z_0) \chi_m(y) \right] \\ &= \sum_{m=1}^{\infty} \chi_m(y_0) \left[\chi_m(y) \frac{d^2}{dz^2} \phi_m(z, z_0) + \phi_m(z, z_0) \chi_m(y) \left\{ k_{ref}^2 - (k_y^{(m)})^2 \right\} \right] \end{aligned} \quad (A.44)$$

Define

$$(k_z^{(m)})^2 = k_{ref}^2 - (k_y^{(m)})^2 \quad (A.45)$$

which brings the **dispersion relation** explicitly in the equation. Therefore,

$$L.H.S = \sum_{m=1}^{\infty} \chi_m(y_0) \left[\chi_m(y) \frac{d^2}{dz^2} \phi_m(z, z_0) + \phi_m(z, z_0) \chi_m(y) (k_z^{(m)})^2 \right] \quad (A.46)$$

$$= \sum_{m=1}^{\infty} \chi_m(y_0) \chi_m(y) \left[\frac{d^2}{dz^2} \phi_m(z, z_0) + (k_z^{(m)})^2 \phi_m(z, z_0) \right] \quad (A.47)$$

Substituting back in equation A.41

$$\sum_{m=1}^{\infty} \chi_m(y_0) \chi_m(y) \left[\frac{d^2}{dz^2} \phi_m(z, z_0) + (k_z^{(m)})^2 \phi_m(z, z_0) \right] = \sum_{m=1}^{\infty} \delta(z - z_0) \chi_m(y_0) \chi_m(y) \quad (A.48)$$

Next, the coefficient of $\chi_m(y_0) \chi_m(y)$ in equation A.48 is compared element-by-element for various m values

$$\frac{d^2}{dz^2} \phi_m(z, z_0) + (k_z^{(m)})^2 \phi_m(z, z_0) = \delta(z - z_0) \quad (A.49)$$

This equation has a familiar form as given in Section A.3.1. On comparing equation A.24 and its solution given in equation A.29 with that of equation A.49,

$$\phi_m(z, z_0) = \frac{1}{2ik_z^{(m)}} e^{ik_z^{(m)}|z-z_0|} \quad (A.50)$$

Substituting back in equation A.38

$$\begin{aligned} G_0(z, y, z_0, y_0) &= \sum_{m=1}^{\infty} \phi_m(z, z_0) \chi_m(y) \chi_m(y_0) \\ &= \sum_{m=1}^{\infty} \frac{1}{2ik_z^{(m)}} e^{ik_z^{(m)}|z-z_0|} \sqrt{\frac{2}{W}} \sin(k_y^{(m)}y) \sqrt{\frac{2}{W}} \sin(k_y^{(m)}y_0) \end{aligned} \quad (\text{A.51})$$

such that $(k_y^{(m)})^2 + (k_z^{(m)})^2 = k_{ref}^2$ and $k_y^{(m)} = m\pi/W$.

A.4 Wave flux or current of eigenmodes $\psi_m(z, y)$

The wave flux density (also called as the wave current density) in the context of Helmholtz equation is defined as (refer page 84 of [30] or [31])

$$\vec{J}_m(z, y) = \frac{1}{2i} \{ \psi_m^* \nabla \psi_m - \psi_m \nabla \psi_m^* \} \quad (\text{A.52})$$

where $\vec{J}_m(z, y)$ denotes the flux density for the m^{th} eigenmode and $*$ denotes complex conjugation. Applying divergence operator $\nabla \cdot$ on the L.H.S and R.H.S of the equation,

$$\begin{aligned} \nabla \cdot \vec{J}_m(z, y) &= \frac{1}{2i} \{ \nabla \cdot (\psi_m^* \nabla \psi_m) - \nabla \cdot (\psi_m \nabla \psi_m^*) \} \\ &= 0 \quad (\text{for proof refer Appendix Section A.5}) \end{aligned} \quad (\text{A.53})$$

gives the steady state continuity equation. Next, evaluating the current density for a right travelling eigenmode (no current along the transverse boundaries) using eq.1.5

$$\begin{aligned} \vec{J}_m(z, y) &= \frac{1}{2i} \{ \psi_m^* \left(\frac{\partial}{\partial z} \psi_m^+ \right) \hat{e}_z - \psi_m^+ \left(\frac{\partial}{\partial z} \psi_m^* \right) \hat{e}_z \} \\ &= \frac{1}{2i} \{ (\Phi_m^+(z)^* \chi_m(y)) \frac{\partial}{\partial z} (\Phi_m^+(z) \chi_m(y)) - (\Phi_m^+(z) \chi_m(y)) \frac{\partial}{\partial z} (\Phi_m^+(z)^* \chi_m(y)) \} \hat{e}_z \\ &= \frac{\chi_m(y)^2}{2i} \{ \Phi_m^+(z)^* \frac{d}{dz} \Phi_m^+(z) - \Phi_m^+(z) \frac{d}{dz} \Phi_m^+(z)^* \} \hat{e}_z \\ &= \frac{\chi_m(y)^2}{2i} \{ \Phi_m^+(z)^* i k_z^{(m)} \Phi_m^+(z) - \Phi_m^+(z) (-i k_z^{(m)}) \Phi_m^+(z)^* \} \hat{e}_z \\ &= \frac{\chi_m(y)^2}{2i} \{ 2i k_z^{(m)} \Phi_m^+(z)^* \Phi_m^+(z) \} \hat{e}_z \end{aligned} \quad (\text{A.54})$$

As $\Phi_m^+(z) = 1/\left(\sqrt{k_z^{(m)}}\right) e^{+ik_z^{(m)}z}$, on substitution

$$\vec{J}_m(z, y) = \frac{\chi_m(y)^2}{2i} \{ 2i k_z^{(m)} \frac{1}{k_z^{(m)}} \} \hat{e}_z = \chi_m(y)^2 \hat{e}_z \quad (\text{A.55})$$

Integrating the flux density $\vec{J}_m(z, y)$ over a given boundary, say Γ_L , net flux crossing the surface along the surface normal, is obtained.

$$flux_m = \int_{\Gamma_L} \vec{J}_m(z, y) \cdot \hat{e}_z dy = \left(\int_{y=0}^{y=W} \chi_m(y)^2 dy \right) \hat{e}_z \cdot \hat{e}_z = 1 \quad \forall m \quad (\because \text{using orthogonality property}) \quad (\text{A.56})$$

This proves that the net current is unity for all eigenmodes and it was obtained by using a normalisation factor of $1/\sqrt{k_z^{(m)}}$ which ensured the net current to be unity for all eigenmodes.

A.5 Continuity equation for current(flux) density

$$\nabla \cdot \vec{J}_m(z, y) = \frac{1}{2i} \{ \nabla \cdot (\psi_m^* \nabla \psi_m) - \nabla \cdot (\psi_m \nabla \psi_m^*) \} \quad (\text{A.57})$$

Using the vector calculus identity that $\nabla \cdot (\phi \nabla \psi) = \phi \nabla^2 \psi + \nabla \phi \cdot \nabla \psi$ where ψ and ϕ are scalar fields, equation A.57 can be expanded as

$$\begin{aligned} \nabla \cdot \vec{J}_m(z, y) &= \frac{1}{2i} [\nabla \cdot (\psi_m^* \nabla \psi_m) - \nabla \cdot (\psi_m \nabla \psi_m^*)] \\ &= \frac{1}{2i} [\{ \psi_m^* \nabla^2 \psi_m + \nabla \psi_m^* \cdot \nabla \psi_m \} - \{ \psi_m \nabla^2 \psi_m^* + \nabla \psi_m \cdot \nabla \psi_m^* \}] \\ &= \frac{1}{2i} \underbrace{[\{ \psi_m^* \nabla^2 \psi_m - \psi_m \nabla^2 \psi_m^* \}]}_{\textcircled{1}} \quad (\because \text{dot products are commutative}) \end{aligned} \quad (\text{A.58})$$

As ψ_m and ψ_m^* obeys Helmholtz equation, multiplying with ψ_m^* and ψ_m as given below

$$\psi_m^* [\nabla^2 + k_{ref}^2] \psi_m = 0 \quad (\text{A.59})$$

$$\psi_m [\nabla^2 + k_{ref}^2] \psi_m^* = 0 \quad (\text{A.60})$$

$$eq.A.59 - eq.A.60 \implies \underbrace{\psi_m^* \nabla^2 \psi_m - \psi_m \nabla^2 \psi_m^*}_{\textcircled{1}} = 0 \implies \nabla \cdot \vec{J}_m(z, y) = 0 \quad (\text{A.61})$$

A.6 Numerical form of eigenmodes $\psi_n^\pm(z_i, y_j)$

Let the discrete version of $\psi_m^+(z_i, y_j)$ on a finite difference grid be written as

$$\psi_m^+(z, y) = \underbrace{c_m^+ e^{+ik_z^{(m)} \Delta_z (z_i - 1)}}_{\Phi_m^+(z_i)} \chi_m(y_j) \quad (\text{A.62})$$

where the real coefficient c_m^+ is assumed to be unknown and $z_i = [1 : N_z]$ in Matlab notation as said before. In this section c_m^+ is solved using the fact that the current injected by all normalised eigenmodes are unity. Reproducing an intermediate step from equation A.54

$$\vec{J}_m(z, y) = \frac{\chi_m(y)^2}{2i} \{ \Phi_m^+(z)^* \frac{d}{dz} \Phi_m^+(z) - \Phi_m^+(z) \frac{d}{dz} \Phi_m^+(z)^* \} \hat{e}_z \quad (\text{A.63})$$

Using the centered first order finite difference formula

$$\frac{d}{dz} \Phi_m^+(z_i) = \frac{\Phi_m^+(z_i + 1) - \Phi_m^+(z_i - 1)}{2\Delta_z}, \quad (\text{A.64})$$

and applying them in the context of equation A.62,

$$\vec{J}_m(z_i, y_j) = \frac{\chi_m(y_j)^2}{2i} \underbrace{\{ \Phi_m^+(z_i)^* \frac{d}{dz} \Phi_m^+(z_i) \}}_{\textcircled{1}} - \underbrace{\{ \Phi_m^+(z_i) \frac{d}{dz} \Phi_m^+(z_i)^* \}}_{\textcircled{2}} \hat{e}_z \quad (\text{A.65})$$

As $\textcircled{2} = \textcircled{1}^*$, solving $\textcircled{1}$ would help for obtaining $\textcircled{2}$

$$\begin{aligned} \textcircled{1} &= \left\{ c_m^+ e^{-ik_z^{(m)} \Delta_z (z_i-1)} \left(\frac{c_m^+ e^{+ik_z^{(m)} \Delta_z (z_i)} - c_m^+ e^{+ik_z^{(m)} \Delta_z (z_i)}}{2\Delta_z} \right) \hat{e}_z \right\} = \left\{ \frac{c_m^{+2} e^{ik_z^{(m)} \Delta_z} - c_m^{+2} e^{-ik_z^{(m)} \Delta_z}}{2\Delta_z} \right\} \hat{e}_z \\ &= i c_m^{+2} \left(\frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z} \right) \hat{e}_z \text{ Hence, } \textcircled{2} = \textcircled{1}^* = -i c_m^{+2} \left(\frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z} \right) \hat{e}_z \end{aligned} \quad (\text{A.66})$$

Substituting back

$$\vec{J}_m(z_i, y_j) = \frac{\chi_m(y_j)^2}{2i} \{\textcircled{1} - \textcircled{2}\} = \frac{\chi_m(y_j)^2}{2i} \left\{ 2i c_m^{+2} \left(\frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z} \right) \hat{e}_z \right\} \quad (\text{A.67})$$

To solve for c_m^+ , the fact that all eigenmodes are normalised to inject a current of unity along the propagating direction, is used. Therefore,

$$flux_m = 1 = \sum_{y_j} \vec{J}_m(z_i, y_j) \cdot \Delta_y \hat{e}_z \quad (\text{A.68})$$

Using discrete numerical orthogonality relationship (equation 1.14) for $\chi_m(y_j)$ when equation A.67 is substituted in equation A.68 yields,

$$\begin{aligned} \sum_{y_j} \vec{J}_m(z_i, y_j) \cdot \Delta_y \vec{n} = 1 &\implies \sum_{y_j} \chi_m(y_j)^2 \Delta_y c_m^{+2} \left(\frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z} \right) = 1 \implies \\ c_m^{+2} \left(\frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z} \right) \underbrace{\sum_{y_j} \chi_m(y_j)^2 \Delta_y}_{=1} &= 1 \implies c_m^+ = \frac{1}{\sqrt{\frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z}}} \end{aligned} \quad (\text{A.69})$$

Substituting for c_m^+ in $\psi_m^+(z_i, y_j)$, discrete form of eigenmodes are obtained

$$\psi_m^+(z_i, y_j) = \frac{1}{\sqrt{\frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z}}} e^{+ik_z^{(m)} \Delta_z (z_i-1)} \chi_m(y_j) \quad (\text{A.70})$$

When $\Delta_z \rightarrow 0$, the continuous analytical form of eigenmode is recovered as

$$\lim_{\Delta_z \rightarrow 0} \frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z} = k_z^{(m)} \quad (\text{A.71})$$

A.7 Dispersion relation using the discretised Helmholtz equation

Consider the analytical scalar Helmholtz equation in 2D for eigenmodes $\psi_m^+(z, y)$

$$[\nabla^2 + k_{ref}^2] \psi_m^+(z, y) = 0 \quad (\text{A.72})$$

In the discretised form, $\nabla^2 \psi_m^+(z, y)$ is given as a centered second order finite difference formula (refer chapter 8.3.2.1 of [109]) acting on $\psi_m^+(z, y)$ (given in equation A.70)

$$\begin{aligned} \nabla^2 \psi_m^+(z_i, y_j) &= \frac{\partial^2}{\partial z^2} \psi_m^+(z_i, y_j) + \frac{\partial^2}{\partial y^2} \psi_m^+(z_i, y_j) \\ &= \underbrace{\frac{\psi_m^+(z_i+1, y_j) - 2\psi_m^+(z_i, y_j) + \psi_m^+(z_i-1, y_j)}{\Delta_z^2}}_{\textcircled{1}} + \underbrace{\frac{\psi_m^+(z_i, y_j+1) - 2\psi_m^+(z_i, y_j) + \psi_m^+(z_i, y_j-1)}{\Delta_y^2}}_{\textcircled{2}} \end{aligned} \quad (\text{A.73})$$

where $z_i = [1 : N_z]$ and $y_i = [1 : N_y]$ are integers in Matlab notation. Substituting the expression for $\psi_m^+(z_i, y_j)$ given in equation A.70, $\textcircled{1}$

$$\begin{aligned} \textcircled{1} &= \frac{1}{\Delta_z^2} \frac{\chi_m(y_j)}{\sqrt{\frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z}}} \left(e^{+ik_z^{(m)} \Delta_z z_i} - 2e^{+ik_z^{(m)} \Delta_z (z_i-1)} + e^{+ik_z^{(m)} \Delta_z (z_i-2)} \right) \\ &= \frac{1}{\Delta_z^2} \underbrace{\frac{\chi_m(y_j) e^{+ik_z^{(m)} \Delta_z (z_i-1)}}{\sqrt{\frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z}}}}_{\psi_m^+(z_i, y_j)} \left(e^{+ik_z^{(m)} \Delta_z} - 2 + e^{-ik_z^{(m)} \Delta_z} \right) \\ &= \frac{1}{\Delta_z^2} \psi_m^+(z_i, y_j) \left\{ 2\cos(k_z^{(m)} \Delta_z) - 2 \right\} = \frac{-1}{\Delta_z^2} \psi_m^+(z_i, y_j) \left(4\sin^2\left(\frac{k_z^{(m)} \Delta_z}{2}\right) \right) \end{aligned} \quad (\text{A.74})$$

Likewise substituting $\psi_m^+(z_i, y_j)$ for evaluating $\textcircled{2}$,

$$\begin{aligned} \textcircled{2} &= \frac{1}{\Delta_y^2} \frac{1}{\sqrt{\frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z}}} e^{+ik_z^{(m)} \Delta_z (z_i-1)} \left\{ \chi_m(y_j+1) - 2\chi_m(y_j) + \chi_m(y_j-1) \right\} \\ &= \frac{1}{\Delta_y^2} \frac{1}{\sqrt{\frac{\sin(k_z^{(m)} \Delta_z)}{\Delta_z}}} e^{+ik_z^{(m)} \Delta_z (z_i-1)} \sqrt{\frac{2}{W}} \underbrace{\left\{ \sin\left(k_y^{(m)} \Delta_y (y_j)\right) - 2\sin\left(k_y^{(m)} \Delta_y (y_j-1)\right) + \sin\left(k_y^{(m)} \Delta_y (y_j-2)\right) \right\}}_{\textcircled{3}} \end{aligned} \quad (\text{A.75})$$

Next, simplify $\textcircled{3}$ using the trigonometric identity $\sin(A) - \sin(B) = 2\sin\left(\frac{A-B}{2}\right)\cos\left(\frac{A+B}{2}\right)$,

$$\begin{aligned} \textcircled{3} &= \sin\left(k_y^{(m)} \Delta_y (y_j)\right) - 2\sin\left(k_y^{(m)} \Delta_y (y_j-1)\right) + \sin\left(k_y^{(m)} \Delta_y (y_j-2)\right) \\ &= \sin\left(k_y^{(m)} \Delta_y (y_j)\right) - \sin\left(k_y^{(m)} \Delta_y (y_j-1)\right) + \sin\left(k_y^{(m)} \Delta_y (y_j-2)\right) - \sin\left(k_y^{(m)} \Delta_y (y_j-1)\right) \\ &= 2\sin\left(\frac{k_y^{(m)} \Delta_y}{2}\right)\cos\left(k_y^{(m)} \Delta_y (y_j) - \frac{k_y^{(m)} \Delta_y}{2}\right) - 2\sin\left(\frac{k_y^{(m)} \Delta_y}{2}\right)\cos\left(k_y^{(m)} \Delta_y (y_j) - \frac{3k_y^{(m)} \Delta_y}{2}\right) \\ &= 2\sin\left(\frac{k_y^{(m)} \Delta_y}{2}\right) \left[\cos\left(k_y^{(m)} \Delta_y (y_j) - \frac{k_y^{(m)} \Delta_y}{2}\right) - \cos\left(k_y^{(m)} \Delta_y (y_j) - \frac{3k_y^{(m)} \Delta_y}{2}\right) \right] \end{aligned} \quad (\text{A.76})$$

Simplifying again using the trigonometric identity $\cos(A) - \cos(B) = 2\sin(\frac{A+B}{2})\sin(\frac{B-A}{2})$,

$$\textcircled{3} = -2\sin\left(\frac{k_y^{(m)}\Delta_y}{2}\right) \left[2\sin\left(k_y^{(m)}\Delta_y(y_j - 1)\right) \sin\left(\frac{k_y^{(m)}\Delta_y}{2}\right) \right] = -4\sin^2\left(\frac{k_y^{(m)}\Delta_y}{2}\right) \sin\left(k_y^{(m)}\Delta_y(y_j - 1)\right) \quad (\text{A.77})$$

Substituting $\textcircled{3}$ in $\textcircled{2}$

$$\begin{aligned} \textcircled{2} &= \frac{-1}{\Delta_y^2} \left(4\sin^2\left(\frac{k_y^{(m)}\Delta_y}{2}\right) \right) \underbrace{\frac{1}{\sqrt{\frac{\sin(k_z^{(m)}\Delta_z)}{\Delta_z}}} e^{+ik_z^{(m)}\Delta_z(z_i-1)} \sqrt{\frac{2}{W}} \left(\sin\left(k_y^{(m)}\Delta_y(y_j - 1)\right) \right)}_{\psi_m^+(z_i, y_j)} \\ &= \frac{-1}{\Delta_y^2} \left(4\sin^2\left(\frac{k_y^{(m)}\Delta_y}{2}\right) \right) \psi_m^+(z_i, y_j) \end{aligned} \quad (\text{A.78})$$

Substituting for $\textcircled{1}$ and $\textcircled{2}$ in equation A.72

$$\frac{-1}{\Delta_z^2} \psi_m^+(z_i, y_j) \left(4\sin^2\left(\frac{k_z^{(m)}\Delta_z}{2}\right) \right) + \frac{-1}{\Delta_y^2} \left(4\sin^2\left(\frac{k_y^{(m)}\Delta_y}{2}\right) \right) \psi_m^+(z_i, y_j) + k_{ref}^2 \psi_m^+(z_i, y_j) = 0 \quad (\text{A.79})$$

This equation implies that for all values of $\psi_m^+(z_i, y_j)$, the equation becomes zero if

$$\frac{4}{\Delta_z^2} \left(\sin^2\left(\frac{k_z^{(m)}\Delta_z}{2}\right) \right) + \frac{4}{\Delta_y^2} \left(\sin^2\left(\frac{k_y^{(m)}\Delta_y}{2}\right) \right) = k_{ref}^2 \quad (\text{A.80})$$

which gives the discretised dispersion relation which on taking the limit $\Delta_z \rightarrow 0$ and $\Delta_y \rightarrow 0$ results in the analytical dispersion relation $\left(k_z^{(m)}\right)^2 + \left(k_y^{(m)}\right)^2 = k_{ref}^2$.

A.8 Numerical solution of the Dyson's equation using the iterative perturbation method

The discretised Dyson's equation is $G_{ij} = G_{ij}^{(0)} + \sum_{k=1}^{k=N_z^P N_y^P} G_{ik}^{(0)} V_k \Delta_{area} G_{kj}$. The entire computational domain which includes the disordered perturbation region and the surrounding region for field visualisation, has the size of $[N_y \times N_z]$. The disorder perturbation region has the size of $[N_y^P \times N_z^P]$, which is a subset of the computational domain $[N_y \times N_z]$. Therefore, there are $N_z^P N_y^P$ scatterer perturbation points. The index i usually denotes the field evaluation location accessed linearly as a 1D array. Similarly, the index j denotes the source location accessed linearly as a 1D array, placed on the boundaries Γ_L or Γ_R . The index k accessed linearly as a 1D array, is associated with the locations at which the scatterer perturbation exists. Two methods are presented as the following where the first method is the direct matrix inversion method. Such a method is easier to understand, but it is memory intensive. The second method is the iterative method which requires iteration steps, but it is memory efficient.

Both the methods start by estimating the free space Green's function $G_{ik}^{(0)}$ and $G_{ij}^{(0)}$, where i spans all the field evaluation points of size $N_y N_z$ for visualisation purposes, k spans all the $N_z^P N_y^P$ scatterer position points where the perturbation is about to be brought in, and j the N_y points associated with the left or the right boundary. $G_{ik}^{(0)}$ is of the dimension $[N_y N_z \times N_y^P N_z^P]$. Other Green's function terms to be appearing in the methods can be derived as a subset from $G_{ik}^{(0)}$ and $G_{ij}^{(0)}$.

A.8.1 Direct method

Step 1 : Using the Dyson's equation, solve for G_{kj} for different locations of $k = k_1, k_2, k_3, \dots, k_{N_z^P N_y^P}$ and a given j location

$$G_{k_1 j} = G_{k_1 j}^{(0)} + \begin{bmatrix} G_{k_1 k_1}^{(0)} V_{k_1} \Delta_{area} & G_{k_1 k_2}^{(0)} V_{k_2} \Delta_{area} & \dots & G_{k_1 k_{N_z^P N_y^P}}^{(0)} V_{k_{N_z^P N_y^P}} \Delta_{area} \end{bmatrix} \begin{pmatrix} G_{k_1 j} \\ G_{k_2 j} \\ \dots \\ G_{k_{(N_z^P N_y^P)} j} \end{pmatrix} \quad (\text{A.81})$$

$$G_{k_2 j} = G_{k_2 j}^{(0)} + \begin{bmatrix} G_{k_2 k_1}^{(0)} V_{k_1} \Delta_{area} & G_{k_2 k_2}^{(0)} V_{k_2} \Delta_{area} & \dots & G_{k_2 k_{N_z^P N_y^P}}^{(0)} V_{k_{N_z^P N_y^P}} \Delta_{area} \end{bmatrix} \begin{pmatrix} G_{k_1 j} \\ G_{k_2 j} \\ \dots \\ G_{k_{(N_z^P N_y^P)} j} \end{pmatrix} \quad (\text{A.82})$$

$\vdots$

$$G_{k_{(N_z^P N_y^P)} j} = G_{k_{(N_z^P N_y^P)} j}^{(0)} + \begin{bmatrix} G_{k_{(N_z^P N_y^P)} k_1}^{(0)} V_{k_1} \Delta_{area} & G_{k_{(N_z^P N_y^P)} k_2}^{(0)} V_{k_2} \Delta_{area} \dots & G_{k_{(N_z^P N_y^P)} k_{N_z^P N_y^P}}^{(0)} V_{k_{N_z^P N_y^P}} \Delta_{area} \end{bmatrix} \begin{pmatrix} G_{k_1 j} \\ G_{k_2 j} \\ \dots \\ G_{k_{(N_z^P N_y^P)} j} \end{pmatrix} \quad (\text{A.83})$$

These set of equations can be written in a matrix form as

$$\begin{pmatrix} G_{k_1 j} \\ G_{k_2 j} \\ G_{k_3 j} \\ \vdots \\ G_{k_{(N_z^P N_y^P)} j} \end{pmatrix} = \begin{pmatrix} G_{k_1 j}^{(0)} \\ G_{k_2 j}^{(0)} \\ G_{k_3 j}^{(0)} \\ \vdots \\ G_{k_{(N_z^P N_y^P)} j}^{(0)} \end{pmatrix} + \underbrace{\begin{pmatrix} G_{k_1 k_1}^{(0)} V_{k_1} & G_{k_1 k_2}^{(0)} V_{k_2} & \dots & G_{k_1 k_{(N_z^P N_y^P)}}^{(0)} V_{k_{(N_z^P N_y^P)}} \\ G_{k_2 k_1}^{(0)} V_{k_1} & G_{k_2 k_2}^{(0)} V_{k_2} & \dots & G_{k_2 k_{(N_z^P N_y^P)}}^{(0)} V_{k_{(N_z^P N_y^P)}} \\ G_{k_3 k_1}^{(0)} V_{k_1} & G_{k_3 k_2}^{(0)} V_{k_2} & \dots & G_{k_3 k_{(N_z^P N_y^P)}}^{(0)} V_{k_{(N_z^P N_y^P)}} \\ \vdots & \vdots & \vdots & \vdots \\ G_{k_{(N_z^P N_y^P)} k_1}^{(0)} V_{k_1} & G_{k_{(N_z^P N_y^P)} k_2}^{(0)} V_{k_2} & \dots & G_{k_{(N_z^P N_y^P)} k_{(N_z^P N_y^P)}}^{(0)} V_{k_{(N_z^P N_y^P)}} \end{pmatrix}}_M \begin{pmatrix} \Delta_{area} G_{k_1 j} \\ \Delta_{area} G_{k_2 j} \\ \Delta_{area} G_{k_3 j} \\ \vdots \\ \Delta_{area} G_{k_{(N_z^P N_y^P)} j} \end{pmatrix} \quad (\text{A.84})$$

Representing the same system of equations as a matrix equation, G_{kj} is solved involving an M matrix (M matrix defined in the above given equation), as given below

$$\begin{aligned} [G_{kj}] &= [G_{kj}^{(0)}] + [M] [G_{kj}] \Rightarrow \\ [G_{kj}] &= [I - [M]]^{-1} [G_{kj}^{(0)}] \end{aligned} \quad (\text{A.85})$$

Step 2 : Once $[G_{kj}]$ is obtained, evaluate $[G_{ij}]$ for a given j

$$\begin{pmatrix} G_{i_1 j} \\ G_{i_2 j} \\ G_{i_3 j} \\ \vdots \\ G_{i_{(N_z N_y)} j} \end{pmatrix} = \begin{pmatrix} G_{i_1 j}^{(0)} \\ G_{i_2 j}^{(0)} \\ G_{i_3 j}^{(0)} \\ \vdots \\ G_{i_{(N_z N_y)} j}^{(0)} \end{pmatrix} + \begin{pmatrix} G_{i_1 k_1}^{(0)} V_{k_1} & G_{i_1 k_2}^{(0)} V_{k_2} & \dots & G_{i_1 k_{(N_z^P N_y^P)}}^{(0)} V_{k_{(N_z^P N_y^P)}} \\ G_{i_2 k_1}^{(0)} V_{k_1} & G_{i_2 k_2}^{(0)} V_{k_2} & \dots & G_{i_2 k_{(N_z^P N_y^P)}}^{(0)} V_{k_{(N_z^P N_y^P)}} \\ G_{i_3 k_1}^{(0)} V_{k_1} & G_{i_3 k_2}^{(0)} V_{k_2} & \dots & G_{i_3 k_{(N_z^P N_y^P)}}^{(0)} V_{k_{(N_z^P N_y^P)}} \\ \vdots & \vdots & \vdots & \vdots \\ G_{i_{(N_z N_y)} k_1}^{(0)} V_{k_1} & G_{i_{(N_z N_y)} k_2}^{(0)} V_{k_2} & \dots & G_{i_{(N_z N_y)} k_{(N_z^P N_y^P)}}^{(0)} V_{k_{(N_z^P N_y^P)}} \end{pmatrix} \begin{pmatrix} \Delta_{area} G_{k_1 j} \\ \Delta_{area} G_{k_2 j} \\ \Delta_{area} G_{k_3 j} \\ \vdots \\ \Delta_{area} G_{k_{(N_z^P N_y^P)} j} \end{pmatrix} \quad (\text{A.86})$$

where there is $N_z N_y$ field evaluation points due to $N_z^P N_y^P$ scattering particles. With step 1 and step 2 evaluated for different source locations j , G_{ij} can be fully solved. Although the direct method presented in this subsection is short and easy to understand, it is memory intensive because of the formation of the large non-sparse M matrix (of size $N_z^P N_y^P \times N_z^P N_y^P$) and the associated inversion process in the equation A.85. Also, the free space Green's function $G_{ik}^{(0)}$ needs to be evaluated for the i corresponding to the entire $[N_z \times N_y]$ grid for the purpose of visualisation. The location k needs to be spanned through all the scattering particle locations (to evaluate the M matrix), consuming memory. To save memory the following iterative method is used instead.

A.8.2 Iterative method involving slices of scatterers

In the iterative method, the total scattering block is divided into slices and the Green's function is updated accounting the scattering effect of the slices taken one at a time. As an example, let's say the entire scattering region is divided into 10 slices. $G_{ik}^{(0)}$ needs to be evaluated like before, for the source k location spanning all the particle positions. $G_{ij}^{(0)}$ is also evaluated where j is on Γ_L or Γ_R . Accounting the scattering perturbation of slice number 1 yields the new updated Green's function $G_{ik}^{(1)}$. While evaluating $G_{ik}^{(1)}$, the source k locations needs to be only those scatterer positions where the remaining 9 slices are to be brought in and also on the boundaries. One could overwrite the $G_{ik}^{(0)}$ array data (only for the source locations of the particles to be brought in, corresponding to the remaining 9 slices) for saving memory. Now the second slice is brought in and $G_{ik}^{(1)}$ is used to evaluate $G_{ik}^{(2)}$ accounting the scattering effect of the second slice. For evaluating $G_{ik}^{(2)}$, the source k locations needs to be only those scatterer locations where the remaining 8 slices are to be brought in and also on the boundaries. The method is repeated by bringing in the remaining slices one by one and updating the Green's function by overwriting the previous version, for the remaining particle positions. Therefore, the process becomes faster upon progressing through the slices.

First, let the first transverse slice of the scatterers be chosen, numbered 1 : N_y^P denoted as $1 \rightarrow N_y^P$. Solve the equation A.84 just for the first slice.

Main step 1 for the iteration method involving the first slice of scatterers

• Sub step 1

$$\begin{aligned}
 \begin{pmatrix} G_{k_1 j}^{(1)} \\ G_{k_2 j}^{(1)} \\ G_{k_3 j}^{(1)} \\ \vdots \\ G_{k_{(N_y^P)} j}^{(1)} \end{pmatrix} &= \begin{pmatrix} G_{k_1 j}^{(0)} \\ G_{k_2 j}^{(0)} \\ G_{k_3 j}^{(0)} \\ \vdots \\ G_{k_{(N_y^P)} j}^{(0)} \end{pmatrix} + \underbrace{\begin{pmatrix} G_{k_1 k_1}^{(0)} V_{k_1} & G_{k_1 k_2}^{(0)} V_{k_2} & \dots & G_{k_1 k_{(N_y^P)}}^{(0)} V_{k_{(N_y^P)}} \\ G_{k_2 k_1}^{(0)} V_{k_1} & G_{k_2 k_2}^{(0)} V_{k_2} & \dots & G_{k_2 k_{(N_y^P)}}^{(0)} V_{k_{(N_y^P)}} \\ G_{k_3 k_1}^{(0)} V_{k_1} & G_{k_3 k_2}^{(0)} V_{k_2} & \dots & G_{k_3 k_{(N_y^P)}}^{(0)} V_{k_{(N_y^P)}} \\ \vdots & \vdots & \vdots & \vdots \\ G_{k_{(N_y^P)} k_1}^{(0)} V_{k_1} & G_{k_{(N_y^P)} k_2}^{(0)} V_{k_2} & \dots & G_{k_{(N_y^P)} k_{(N_y^P)}}^{(0)} V_{k_{(N_y^P)}} \end{pmatrix}}_{M_{(1 \rightarrow N_y^P)}^{(0)}} \begin{pmatrix} \Delta_{area} G_{k_1 j}^{(1)} \\ \Delta_{area} G_{k_2 j}^{(1)} \\ \Delta_{area} G_{k_3 j}^{(1)} \\ \vdots \\ \Delta_{area} G_{k_{(N_y^P)} j}^{(1)} \end{pmatrix} \quad (\text{A.87})
 \end{aligned}$$

- **Sub step 2** Representing the above given system of equations as a matrix equation, $G_{k_{(1 \rightarrow N_y^p)}j}^{(1)}$ is solved involving the $M_{(1 \rightarrow N_y^p)}^{(0)}$ matrix (defined in the previous equation), as given below

$$\begin{aligned} \begin{bmatrix} G_{k_{(1 \rightarrow N_y^p)}j}^{(1)} \end{bmatrix} &= \begin{bmatrix} G_{k_{(1 \rightarrow N_y^p)}j}^{(0)} \end{bmatrix} + \begin{bmatrix} M_{(1 \rightarrow N_y^p)}^{(0)} \end{bmatrix} \begin{bmatrix} G_{k_{(1 \rightarrow N_y^p)}j}^{(1)} \end{bmatrix} \Rightarrow \\ \begin{bmatrix} G_{k_{(1 \rightarrow N_y^p)}j}^{(1)} \end{bmatrix} &= \left[I - \begin{bmatrix} M_{(1 \rightarrow N_y^p)}^{(0)} \end{bmatrix} \right]^{-1} \begin{bmatrix} G_{k_{(1 \rightarrow N_y^p)}j}^{(0)} \end{bmatrix} \end{aligned} \quad (\text{A.88})$$

- **Sub step 3** Once $[G_{k_{(1 \rightarrow N_y^p)}j}^{(1)}]$ is obtained, evaluate $[G_{ij}^{(1)}]$ for a given j

$$\begin{aligned} \begin{bmatrix} G_{i_1j}^{(1)} \\ G_{i_2j}^{(1)} \\ G_{i_3j}^{(1)} \\ \vdots \\ G_{i_{(N_z N_y)}j}^{(1)} \end{bmatrix} &= \begin{bmatrix} G_{i_1j}^{(0)} \\ G_{i_2j}^{(0)} \\ G_{i_3j}^{(0)} \\ \vdots \\ G_{i_{(N_z N_y)}j}^{(0)} \end{bmatrix} + \begin{pmatrix} G_{i_1k_1}^{(0)} V_{k_1} & G_{i_1k_2}^{(0)} V_{k_2} & \dots & G_{i_1k_{(N_y^p)}}^{(0)} V_{k_{(N_y^p)}} \\ G_{i_2k_1}^{(0)} V_{k_1} & G_{i_2k_2}^{(0)} V_{k_2} & \dots & G_{i_2k_{(N_y^p)}}^{(0)} V_{k_{(N_y^p)}} \\ G_{i_3k_1}^{(0)} V_{k_1} & G_{i_3k_2}^{(0)} V_{k_2} & \dots & G_{i_3k_{(N_y^p)}}^{(0)} V_{k_{(N_y^p)}} \\ \vdots & \vdots & \vdots & \vdots \\ G_{i_{(N_z N_y)}k_1}^{(0)} V_{k_1} & G_{i_{(N_z N_y)}k_2}^{(0)} V_{k_2} & \dots & G_{i_{(N_z N_y)}k_{(N_y^p)}}^{(0)} V_{k_{(N_y^p)}} \end{pmatrix} \begin{pmatrix} \Delta_{area} G_{k_1j}^{(1)} \\ \Delta_{area} G_{k_2j}^{(1)} \\ \Delta_{area} G_{k_3j}^{(1)} \\ \vdots \\ \Delta_{area} G_{k_{(N_y^p)}j}^{(1)} \end{pmatrix} \end{aligned} \quad (\text{A.89})$$

- **Sub step 4** Before moving onto the next main iteration step (main iteration step number 2), the following sub step evaluations has to be performed to estimate $[G_{k_{(1 \rightarrow N_y^p)}k_{(N_y^p+1 \rightarrow N_y^p N_z^p)}}^{(1)}]$ and $[G_{ik_{(N_y^p+1 \rightarrow N_y^p N_z^p)}}^{(1)}]$ to be used in the next main iteration step. Here $(N_y^p + 1 \rightarrow N_y^p N_z^p)$ corresponds to the remaining scatter position where the perturbation is brought-in in the future iteration steps by introducing slice number 2,3,4 etc..

Using equation A.88,

$$\begin{bmatrix} G_{k_{(1 \rightarrow N_y^p)}k_{(N_y^p+1 \rightarrow N_y^p N_z^p)}}^{(1)} \end{bmatrix} = \left[I - \begin{bmatrix} M_{(1 \rightarrow N_y^p)}^{(0)} \end{bmatrix} \right]^{-1} \begin{bmatrix} G_{k_{(1 \rightarrow N_y^p)}k_{(N_y^p+1 \rightarrow N_y^p N_z^p)}}^{(0)} \end{bmatrix} \quad (\text{A.90})$$

Taking equation A.89 and substituting for j as $k_{(N_y^p+1 \rightarrow N_y^p N_z^p)}$, together with the above given equation, $[G_{ik_{(N_y^p+1 \rightarrow N_y^p N_z^p)}}^{(1)}]$ can be estimated. The estimated $[G_{ik_{(N_y^p+1 \rightarrow N_y^p N_z^p)}}^{(1)}]$ can be overwritten upon the existing memory taken by $G_{ik}^{(0)}$.

Main step 2 involving the second slice of scatterers denoted by $N_y^p + 1 \rightarrow 2N_y^p$,

- **Sub step 1**

$$\begin{aligned} \begin{bmatrix} G_{k_{(N_y^p+1)}j}^{(2)} \\ G_{k_{(N_y^p+2)}j}^{(2)} \\ G_{k_{(N_y^p+3)}j}^{(2)} \\ \vdots \\ G_{k_{(2N_y^p)}j}^{(2)} \end{bmatrix} &= \begin{bmatrix} G_{k_{(N_y^p+1)}j}^{(1)} \\ G_{k_{(N_y^p+2)}j}^{(1)} \\ G_{k_{(N_y^p+3)}j}^{(1)} \\ \vdots \\ G_{k_{(2N_y^p)}j}^{(1)} \end{bmatrix} + \underbrace{\begin{pmatrix} G_{k_{(N_y^p+1)}k_{(N_y^p+1)}}^{(1)} V_{k_{(N_y^p+1)}} & G_{k_{(N_y^p+1)}k_{(N_y^p+2)}}^{(1)} V_{k_{(N_y^p+2)}} & \dots & G_{k_{(N_y^p+1)}k_{(2N_y^p)}}^{(1)} V_{k_{(2N_y^p)}} \\ G_{k_{(N_y^p+2)}k_{(N_y^p+1)}}^{(1)} V_{k_{(N_y^p+1)}} & G_{k_{(N_y^p+2)}k_{(N_y^p+2)}}^{(1)} V_{k_{(N_y^p+2)}} & \dots & G_{k_{(N_y^p+2)}k_{(2N_y^p)}}^{(1)} V_{k_{(2N_y^p)}} \\ G_{k_{(N_y^p+3)}k_{(N_y^p+1)}}^{(1)} V_{k_{(N_y^p+1)}} & G_{k_{(N_y^p+3)}k_{(N_y^p+2)}}^{(1)} V_{k_{(N_y^p+2)}} & \dots & G_{k_{(N_y^p+3)}k_{(2N_y^p)}}^{(1)} V_{k_{(2N_y^p)}} \\ \vdots & \vdots & \vdots & \vdots \\ G_{k_{(2N_y^p)}k_{(N_y^p+1)}}^{(1)} V_{k_{(N_y^p+1)}} & G_{k_{(2N_y^p)}k_{(N_y^p+2)}}^{(1)} V_{k_{(N_y^p+2)}} & \dots & G_{k_{(2N_y^p)}k_{(2N_y^p)}}^{(1)} V_{k_{(2N_y^p)}} \end{pmatrix}}_{M_{(N_y^p+1 \rightarrow 2N_y^p)}^{(1)}} \begin{pmatrix} \Delta_{area} G_{k_{(N_y^p+1)}j}^{(2)} \\ \Delta_{area} G_{k_{(N_y^p+2)}j}^{(2)} \\ \Delta_{area} G_{k_{(N_y^p+3)}j}^{(2)} \\ \vdots \\ \Delta_{area} G_{k_{(2N_y^p)}j}^{(2)} \end{pmatrix} \end{aligned}$$

- **Sub step 2** Representing the above given system of equations as a matrix equation, $G_{k_{(N_y^p+1 \rightarrow 2N_y^p)}j}^{(2)}$ is solved involving the $M_{(N_y^p+1 \rightarrow 2N_y^p)}^{(1)}$ matrix (defined in the previous equation), as given below

$$\begin{aligned} \begin{bmatrix} G_{k_{(N_y^p+1 \rightarrow 2N_y^p)}j}^{(2)} \end{bmatrix} &= \begin{bmatrix} G_{k_{(N_y^p+1 \rightarrow 2N_y^p)}j}^{(1)} \end{bmatrix} + \begin{bmatrix} M_{(N_y^p+1 \rightarrow 2N_y^p)}^{(1)} \end{bmatrix} \begin{bmatrix} G_{k_{(N_y^p+1 \rightarrow 2N_y^p)}j}^{(2)} \end{bmatrix} \Rightarrow \\ \begin{bmatrix} G_{k_{(N_y^p+1 \rightarrow 2N_y^p)}j}^{(2)} \end{bmatrix} &= \left[I - \begin{bmatrix} M_{(N_y^p+1 \rightarrow 2N_y^p)}^{(1)} \end{bmatrix} \right]^{-1} \begin{bmatrix} G_{k_{(N_y^p+1 \rightarrow 2N_y^p)}j}^{(1)} \end{bmatrix} \end{aligned} \quad (\text{A.91})$$

- **Sub step 3** Once $[G_{k_{(N_y^p+1 \rightarrow 2N_y^p)}j}^{(2)}]$ is obtained, evaluate $[G_{ij}^{(2)}]$ for a given j .

$$\begin{aligned} \begin{bmatrix} G_{i_1j}^{(2)} \\ G_{i_2j}^{(2)} \\ G_{i_3j}^{(2)} \\ \vdots \\ G_{i_{(N_z N_y)}j}^{(2)} \end{bmatrix} &= \begin{bmatrix} G_{i_1j}^{(1)} \\ G_{i_2j}^{(1)} \\ G_{i_3j}^{(1)} \\ \vdots \\ G_{i_{(N_z N_y)}j}^{(1)} \end{bmatrix} + \begin{pmatrix} G_{i_1k_{(N_y^p+1)}}^{(1)} V_{k_{(N_y^p+1)}} & G_{i_1k_{(N_y^p+2)}}^{(1)} V_{k_{(N_y^p+2)}} & \dots & G_{i_1k_{(2N_y^p)}}^{(1)} V_{k_{(2N_y^p)}} \\ G_{i_2k_{(N_y^p+1)}}^{(1)} V_{k_{(N_y^p+1)}} & G_{i_2k_{(N_y^p+2)}}^{(1)} V_{k_{(N_y^p+2)}} & \dots & G_{i_2k_{(2N_y^p)}}^{(1)} V_{k_{(2N_y^p)}} \\ G_{i_3k_{(N_y^p+1)}}^{(1)} V_{k_{(N_y^p+1)}} & G_{i_3k_{(N_y^p+2)}}^{(1)} V_{k_{(N_y^p+2)}} & \dots & G_{i_3k_{(2N_y^p)}}^{(1)} V_{k_{(2N_y^p)}} \\ \vdots & \vdots & \vdots & \vdots \\ G_{i_{(N_z N_y)}k_{(N_y^p+1)}}^{(1)} V_{k_{(N_y^p+1)}} & G_{i_{(N_z N_y)}k_{(N_y^p+2)}}^{(1)} V_{k_{(N_y^p+2)}} & \dots & G_{i_{(N_z N_y)}k_{(2N_y^p)}}^{(1)} V_{k_{(2N_y^p)}} \end{pmatrix} \begin{pmatrix} \Delta_{area} G_{k_{(N_y^p+1)}j}^{(2)} \\ \Delta_{area} G_{k_{(N_y^p+2)}j}^{(2)} \\ \Delta_{area} G_{k_{(N_y^p+3)}j}^{(2)} \\ \vdots \\ \Delta_{area} G_{k_{(2N_y^p)}j}^{(2)} \end{pmatrix} \end{aligned} \quad (\text{A.92})$$

- **Sub step 4** Before moving onto the next main iteration step (main iteration step number 3), the following sub step evaluations has to be performed to estimate $[G_{k_{(N_y^p+1 \rightarrow 2N_y^p)}k_{(2N_y^p+1 \rightarrow N_y^p N_z^p)}}^{(2)}]$ and $[G_{ik_{(2N_y^p+1 \rightarrow N_y^p N_z^p)}}^{(2)}]$ to be used in the next main iteration step. Here $(2N_y^p + 1 \rightarrow N_y^p N_z^p)$ corresponds to the remaining scatter position where the perturbation is brought-in in the future iteration steps by introducing slice number 3,4,5 etc..

Using equation A.91,

$$\begin{bmatrix} G_{k_{(N_y^p+1 \rightarrow 2N_y^p)}k_{(2N_y^p+1 \rightarrow N_y^p N_z^p)}}^{(2)} \end{bmatrix} = \left[I - \begin{bmatrix} M_{(N_y^p+1 \rightarrow 2N_y^p)}^{(1)} \end{bmatrix} \right]^{-1} \begin{bmatrix} G_{k_{(N_y^p+1 \rightarrow 2N_y^p)}k_{(2N_y^p+1 \rightarrow N_y^p N_z^p)}}^{(1)} \end{bmatrix} \quad (\text{A.93})$$

Taking equation A.92 and substituting for j as $k_{(2N_y^p+1 \rightarrow N_y^p N_z^p)}$, together with the above given equation, $[G_{ik_{(2N_y^p+1 \rightarrow N_y^p N_z^p)}}^{(2)}]$ can be estimated. The estimated $[G_{ik_{(2N_y^p+1 \rightarrow N_y^p N_z^p)}}^{(2)}]$ can be overwritten upon the existing memory taken by $G_{ik}^{(1)}$.

Following the same logic, the main step 3 involving the slice of scatterers denoted by $2N_y^p + 1 \rightarrow 3N_y^p$ can be evaluated. The iteration process continues until the last slice of scatterers are brought in, obtaining the fully perturbed Green's function G_{ij} .

A.9 Green's second identity and eigenmodes

Let $\psi_m^+(z, y)$ and $\psi_n^+(z, y)$ are two eigenmodes satisfying the homogeneous boundary conditions given in 1.27. Green's second identity in general is given as

$$\begin{aligned} \int \int \{ \psi_m^+ \nabla^2 \psi_n^+ - \psi_n^+ \nabla^2 \psi_m^+ \} dz dy &= \int \int \nabla \cdot \{ \psi_m^+ \nabla \psi_n^+ - \psi_n^+ \nabla \psi_m^+ \} dz dy \\ &= \int_{\Gamma} \{ \psi_m^+ \nabla \psi_n^+ - \psi_n^+ \nabla \psi_m^+ \} \cdot \vec{n} d\Gamma \end{aligned} \quad (\text{A.94})$$

where the double integral on the *L.H.S* operates on the region Ω enclosed by the boundary Γ as shown in the Figure 1.2. *R.H.S* of the above given equation is the boundary integral for evaluating the flux crossing the entire boundary due to the integrand. As we know that there is no flux crossing along the transverse boundaries, hence only the boundary integral along Γ_L and Γ_R need to be evaluated. In addition to that, only the d/dz component of ∇ needs to be evaluated as it is the only component along the direction of $\vec{n}$ ($\vec{n}$ points outwards of the sample as shown in the Figure 1.2). Therefore,

$$\begin{aligned} \int_{\Gamma} \{ \psi_m^+ \nabla \psi_n^+ - \psi_n^+ \nabla \psi_m^+ \} \cdot \vec{n} d\Gamma &= \underbrace{\int \left\{ \psi_m^+ \left(\frac{\partial}{\partial z} \psi_n^+ \right) \hat{e}_z - \psi_n^+ \left(\frac{\partial}{\partial z} \psi_m^+ \right) \hat{e}_z \right\} \cdot (-\hat{e}_z dy) |_{(z,y) \in \Gamma_L} +}_{\textcircled{1}} \\ &\underbrace{\int \left\{ \psi_m^+ \left(\frac{\partial}{\partial z} \psi_n^+ \right) \hat{e}_z - \psi_n^+ \left(\frac{\partial}{\partial z} \psi_m^+ \right) \hat{e}_z \right\} \cdot (+\hat{e}_z dy) |_{(z,y) \in \Gamma_R}}_{\textcircled{2}} \end{aligned} \quad (\text{A.95})$$

If $m \neq n$, then $\textcircled{1} = \textcircled{2} = 0$, because of the orthogonality relationship $\langle \chi_m | \chi_n \rangle = 0$ as ψ_m^+ and ψ_n^+ contain functions χ_m and χ_n , respectively. Now, consider the case when $m = n$ and hence, $k_z^{(n)} = k_z^{(m)}$. Therefore, once again it can be seen that $\textcircled{1} = \textcircled{2} = 0$. Therefore,

$$\int \int \{ \psi_m^+ \nabla^2 \psi_n^+ - \psi_n^+ \nabla^2 \psi_m^+ \} dz dy = \int_{\Gamma} \{ \psi_m^+ \nabla \psi_n^+ - \psi_n^+ \nabla \psi_m^+ \} \cdot \vec{n} d\Gamma = 0 \quad (\text{A.96})$$

A.10 Reciprocity of perturbed Green's function, $G(r, r_0)$

Consider the following Green's function equations for two different Dirac delta sources at r_1 and r_2

$$\nabla_r^2 G(r, r_1) + k_0^2 \epsilon_r(r) G(r, r_1) = \delta(r - r_1) \quad (\text{A.97})$$

$$\nabla_r^2 G(r, r_2) + k_0^2 \epsilon_r(r) G(r, r_2) = \delta(r - r_2) \quad (\text{A.98})$$

Multiplying the above equations using $G(r, r_2)$ and $G(r, r_1)$

$$G(r, r_2) \nabla_r^2 G(r, r_1) + k_0^2 \epsilon_r(r) G(r, r_1) G(r, r_2) = G(r, r_2) \delta(r - r_1) \quad (\text{A.99})$$

$$G(r, r_1) \nabla_r^2 G(r, r_2) + k_0^2 \epsilon_r(r) G(r, r_1) G(r, r_2) = G(r, r_1) \delta(r - r_2) \quad (\text{A.100})$$

Integrating over the region Ω

$$\int \int \{ G(r, r_2) \nabla_r^2 G(r, r_1) + k_0^2 \epsilon_r(r) G(r, r_1) G(r, r_2) \} dz dy = \int \int G(r, r_2) \delta(r - r_1) dz dy \quad (\text{A.101})$$

$$\int \int \{ G(r, r_1) \nabla_r^2 G(r, r_2) + k_0^2 \epsilon_r(r) G(r, r_1) G(r, r_2) \} dz dy = \int \int G(r, r_1) \delta(r - r_2) dz dy \quad (\text{A.102})$$

Using the sifting property of Dirac delta function on the *R.H.S* of the above given equations, followed by subtraction, the following is obtained

$$\int \int \{ G(r, r_2) \nabla_r^2 G(r, r_1) - G(r, r_1) \nabla_r^2 G(r, r_2) \} dz dy = G(r_1, r_2) - G(r_2, r_1) \quad (\text{A.103})$$

Next, the goal would be to relate the above given equation with that of equation A.96. The perturbed Green's function can be decomposed in terms of outgoing eigemodes ψ_m^+ and ψ_m^- at the boundaries as given in equations 1.45 and 1.46. In addition to that $G(r, r_1)$ and $G(r, r_2)$ obey homogeneous boundary conditions as given in equation 1.47 and 1.48. Considering these facts and following the same logic as given in Section A.9, one could show that the *L.H.S* of equation A.103 is zero. Hence,

$$G(r_1, r_2) - G(r_2, r_1) = 0 \implies G(r_1, r_2) = G(r_2, r_1) \quad (\text{A.104})$$

A.11 Derivation of generalised Fisher-Lee relationships

Generalised Fisher-Lee relations are obtained by substituting expression for the total field $E(z_0, y_0)$ in the BI equation and solving for the reflection or transmission coefficients.

A.11.1 Derivation for S_{11}

First, let the wave incidence be from the left side of the disorder onto Γ_L . For estimating the reflection matrix S_{11} need to take $(z_0, y_0) \in \Gamma_L$. Then the simplified boundary integral equation becomes,

$$\begin{aligned} & \sum_{m=1}^{M_{total}} 2ik_z^{(m)} \int E_m^{inc}(z, y) G(z, y, z_0, y_0) dy|_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_L} = E(z_0, y_0)|_{(z_0,y_0) \in \Gamma_L} \\ & = \sum_{n=1}^{N_{total}} E_n(z_0, y_0)|_{(z_0,y_0) \in \Gamma_L} \\ & = \sum_{m=1}^{M_{total}} \sum_{n=1}^{N_{total}} c_m^+ [\delta_{kron}(n, m) \chi_n(y_0) \phi_n^+(z_0) + S_{11}^{nm} \chi_n(y_0) \phi_n^-(z_0)]|_{(z_0,y_0) \in \Gamma_L} \end{aligned} \quad (A.105)$$

Comparing the summation terms covered by $\sum_{m=1}^{M_{total}}$ on *L.H.S* and *R.H.S*,

$$\begin{aligned} & 2ik_z^{(m)} c_m^+ \phi_m^+(z) \int \chi_m(y) G(z, y, z_0, y_0) dy|_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_L} = \\ & \sum_{n=1}^{N_{total}} c_m^+ [\delta_{kron}(n, m) \phi_n^+(z_0) \chi_n(y_0) + S_{11}^{nm} \chi_n(y_0) \phi_n^-(z_0)]|_{(z_0,y_0) \in \Gamma_L} \end{aligned} \quad (A.106)$$

Using the orthogonality relationship involving $\chi'_n(y)$ and integrating with respect to y_0 on both sides of the above given equation,

$$\begin{aligned} & 2ik_z^{(m)} \phi_m^+(z) c_m^+ \int_{y_0} \int_y \chi_m(y) G(z, y, z_0, y_0) \chi_{n'}(y_0) dy dy_0|_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_L} = \\ & \int_{y_0} \chi_{n'}(y_0) \left\{ \sum_{n=1}^{N_{total}} c_m^+ [\delta_{kron}(n, m) \phi_n^+(z_0) \chi_n(y_0) + S_{11}^{nm} \chi_n(y_0) \phi_n^-(z_0)] dy_0 \right\}|_{(z_0,y_0) \in \Gamma_L} \\ & = c_m^+ \{ \delta_{kron}(n', m) \phi_{n'}^+(z_0) + S_{11}^{mn'} \phi_{n'}^-(z_0) \} \end{aligned} \quad (A.107)$$

On comparing the coefficients of c_m^+ on *L.H.S* and *R.H.S* of the previous equation,

$$\begin{aligned} & 2ik_z^{(m)} \phi_m^+(z) \int_{y_0} \int_y \chi_m(y) G(z, y, z_0, y_0) \chi_{n'}(y_0)|_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_L} dy dy_0 = \\ & \delta_{kron}(n', m) \phi_{n'}^+(z_0) + S_{11}^{mn'} \phi_{n'}^-(z_0) \end{aligned} \quad (A.108)$$

Simplification : Rename n' as n and let z and z_0 be positioned at 0 on the left boundary. Therefore,

$$\begin{aligned} & 2ik_z^{(m)} \phi_m^+(z=0) \int_{y_0} \int_y \chi_m(y) G(z=0, y, z_0=0, y_0) \chi_n(y_0)|_{(z=0,y) \in \Gamma_L \& (z_0=0,y_0) \in \Gamma_L} dy dy_0 = \\ & \delta_{kron}(n, m) \phi_n^+(z_0=0) + S_{11}^{nm} \phi_n^-(z_0=0) \end{aligned} \quad (A.109)$$

Mathematically, there are 4 different possibilities with respect to the nature of incident and reflected modes.

Case 1 : Both input and output modes are propagating $m \leq M_{prop}$ and $n \leq N_{prop}$

$$2ik_z^{(m)} \frac{1}{\sqrt{k_z^{(m)}}} \int_{y_0} \int_y \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) |_{(z=0, y) \in \Gamma_L \& (z_0=0, y_0) \in \Gamma_L} dy dy_0 = \delta_{\text{kron}}(n, m) \frac{1}{\sqrt{k_z^{(n)}}} + \frac{S_{11}^{nm}}{\sqrt{k_z^{(n)}}} \quad (\text{A.110})$$

Case 2 : Input mode and output modes are evanescent $m > M_{\text{prop}}$ and $n > N_{\text{prop}}$

$$2ik_z^{(m)} \frac{1}{\sqrt{|k_z^{(m)}|}} \int_{y_0} \int_y \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) |_{(z=0, y) \in \Gamma_L \& (z_0=0, y_0) \in \Gamma_L} dy dy_0 = \delta_{\text{kron}}(n, m) \frac{1}{\sqrt{|k_z^{(n)}|}} + S_{11}^{nm} \frac{1}{\sqrt{|k_z^{(n)}|}} \quad (\text{A.111})$$

Case 3 : Input modes are propagating and output modes are evanescent $m \leq M_{\text{prop}}$ and $n > N_{\text{prop}}$

$$2ik_z^{(m)} \frac{1}{\sqrt{k_z^{(m)}}} \int_{y_0} \int_y \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) |_{(z=0, y) \in \Gamma_L \& (z_0=0, y_0) \in \Gamma_L} dy dy_0 = \delta_{\text{kron}}(n, m) \frac{1}{\sqrt{k_z^{(n)}}} + S_{11}^{nm} \frac{1}{\sqrt{|k_z^{(n)}|}} \quad (\text{A.112})$$

But $\delta_{\text{kron}}(n, m) = 0$, if $m \leq M_{\text{prop}}$ and $n > N_{\text{prop}}$

Case 4 : Input modes are evanescent and output modes are propagating $m > M_{\text{prop}}$ and $n \leq N_{\text{prop}}$

$$2ik_z^{(m)} \frac{1}{\sqrt{|k_z^{(m)}|}} \int_{y_0} \int_y \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) |_{(z=0, y) \in \Gamma_L \& (z_0=0, y_0) \in \Gamma_L} dy dy_0 = \delta_{\text{kron}}(n, m) \frac{1}{\sqrt{|k_z^{(n)}|}} + S_{11}^{mn} \frac{1}{\sqrt{k_z^{(n)}}} \quad (\text{A.113})$$

But $\delta_{\text{kron}}(n, m) = 0$, if $m > M_{\text{prop}}$ and $n \leq N_{\text{prop}}$.

Solving for S_{11} for cases 1, 2, 3 and 4, (using the information that for evanescent modes $\frac{k_z^{(m)}}{\sqrt{|k_z^{(m)}|}} = i\sqrt{|k_z^{(m)}|}$, is imaginary) are summarised in the Table 1.1.

A.11.2 Derivation for S_{21}

Let the wave incidence be from the left side of the disorder onto Γ_L . For estimating the transmission matrix S_{21} , need to take $(z_0, y_0) \in \Gamma_R$. Then the simplified boundary integral equation becomes,

$$\begin{aligned} & \sum_{m=1}^{M_{\text{total}}} 2ik_z^{(m)} \int E_m^{\text{inc}}(z, y) G(z, y, z_0, y_0) dy |_{(z, y) \in \Gamma_L \& (z_0, y_0) \in \Gamma_R} = E(z_0, y_0) |_{(z_0, y_0) \in \Gamma_R} \\ &= \sum_{n=1}^{N_{\text{total}}} E_n(z_0, y_0) |_{(z_0, y_0) \in \Gamma_R} = \sum_{n=1}^{N_{\text{total}}} t_n^+ \chi_n(y_0) \phi_n^+(z_0) |_{(z_0, y_0) \in \Gamma_R} \\ &= \sum_{n=1}^{N_{\text{total}}} \left\{ \sum_{m=1}^{M_{\text{total}}} c_m^+ S_{21}^{nm} \right\} \chi_n(y_0) \phi_n^+(z_0) |_{(z_0, y_0) \in \Gamma_R} \end{aligned} \quad (\text{A.114})$$

Comparing the summation terms covered by $\sum_{m=1}^{M_{\text{total}}}$ on *L.H.S* and *R.H.S*,

$$2ik_z^{(m)} \int c_m^+ \phi_m^+(z) \chi_m(y) G(z, y, z_0, y_0) dy |_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_R} = \sum_{n=1}^{N_{\text{total}}} c_m^+ S_{21}^{nm} \chi_n(y_0) \phi_n^+(z_0) |_{(z_0,y_0) \in \Gamma_R} \quad (\text{A.115})$$

Using the orthogonality relationship involving $\chi_{n'}(y)$ and integrating with respect to y_0 on both sides of the above given equation,

$$2ik_z^{(m)} c_m^+ \phi_m^+(z) \int_y \int_{y_0} \chi_m(y) G(z, y, z_0, y_0) \chi_{n'}(y_0) dy dy_0 |_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_R} = c_m^+ S_{21}^{n'm} \phi_{n'}^+(z_0) |_{z_0 \in \Gamma_R} \quad (\text{A.116})$$

On comparing the coefficients of c_m^+ on *L.H.S* and *R.H.S* of the previous equation,

$$2ik_z^{(m)} \phi_m^+(z) \int_y \int_{y_0} \chi_m(y) G(z, y, z_0, y_0) \chi_{n'}(y_0) dy dy_0 |_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_R} = S_{21}^{n'm} \phi_{n'}^+(z_0) |_{z_0 \in \Gamma_R} \quad (\text{A.117})$$

Simplification : Rename n' as n and let z be positioned at 0 on the left boundary and $z_0 = z_R$ at Γ_R on the right boundary. Therefore,

$$2ik_z^{(m)} \phi_m^+(z=0) \int_y \int_{y_0} \chi_m(y) G(z=0, y, z_0=z_R, y_0) \chi_n(y_0) dy dy_0 |_{(z=0,y) \in \Gamma_L \& (z_0=z_R,y_0) \in \Gamma_R} = S_{21}^{nm} \phi_n^+(z_0=z_R) |_{(z_0=z_R) \in \Gamma_R} \quad (\text{A.118})$$

Mathematically, there are 4 different possibilities with respect to the nature of incident and transmitted modes.

Case 1 : Both input and output modes are propagating $m \leq M_{\text{prop}}$ and $n \leq N_{\text{prop}}$

$$2ik_z^{(m)} \frac{1}{\sqrt{k_z^{(m)}}} \int_y \int_{y_0} \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) dy dy_0 |_{(z=0,y) \in \Gamma_L \& (z_0=z_R,y_0) \in \Gamma_R} = S_{21}^{nm} \frac{1}{\sqrt{k_z^{(n)}}} e^{+ik_z^{(n)} z_R} \quad (\text{A.119})$$

Case 2 : Input mode and output modes are evanescent $m > M_{\text{prop}}$ and $n > N_{\text{prop}}$

$$2ik_z^{(m)} \frac{1}{\sqrt{|k_z^{(m)}|}} \int_y \int_{y_0} \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) dy dy_0 |_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_R} = S_{21}^{nm} \frac{1}{\sqrt{|k_z^{(n)}|}} \quad (\text{A.120})$$

Case 3 : Input modes are propagating and output modes are evanescent $m \leq M_{\text{prop}}$ and $n > N_{\text{prop}}$

$$2ik_z^{(m)} \frac{1}{\sqrt{k_z^{(m)}}} \int_y \int_{y_0} \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) dy dy_0 |_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_R} = S_{21}^{nm} \frac{1}{\sqrt{|k_z^{(n)}|}} \quad (\text{A.121})$$

Case 4 : Input modes are evanescent and output modes are propagating $m > M_{\text{prop}}$ and $n \leq N_{\text{prop}}$

$$2ik_z^{(m)} \frac{1}{\sqrt{|k_z^{(m)}|}} \int_y \int_{y_0} \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) dy dy_0 |_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_R} = S_{21}^{nm} \frac{e^{+iz_R k_z^{(n)}}}{\sqrt{k_z^{(n)}}} \quad (\text{A.122})$$

Solving for S_{21} for cases 1, 2, 3 and 4 (using the information that for evanescent modes $\frac{k_z^{(m)}}{\sqrt{|k_z^{(m)}|}} = i\sqrt{|k_z^{(m)}|}$, is imaginary) are summarised in the Table 1.2.

A.11.3 Derivation for S_{22}

Let the wave incidence be from the right side of the disorder onto Γ_R . For estimating the reflection matrix S_{22} , need to take $(z_0, y_0) \in \Gamma_R$. Then the simplified boundary integral equation becomes,

$$\begin{aligned} \sum_{m=1}^{M_{total}} 2ik_z^{(m)} \int E_m^{inc}(z, y) G(z, y, z_0, y_0) dy |_{(z,y) \in \Gamma_R \& (z_0,y_0) \in \Gamma_R} &= \sum_{n=1}^{N_{total}} E_n(z_0, y_0) |_{(z_0,y_0) \in \Gamma_R} \\ &= \sum_{m=1}^{M_{total}} \sum_{n=1}^{N_{total}} c_m^- [\delta_{kron}(n, m) \phi_n^-(z_0) \chi_n(y_0) + S_{22}^{nm} \chi_n(y_0) \phi_n^+(z_0)] |_{(z_0,y_0) \in \Gamma_R} \end{aligned} \quad (A.123)$$

Performing the same set of operations as used for the derivation of S_{11} and setting $z = z_R$ and $z_0 = z_R$, the following is obtained

$$\begin{aligned} 2ik_z^{(m)} \phi_m^-(z = z_R) \int_{y_0} \int_y \chi_m(y) G(z = z_R, y, z_0 = z_R, y_0) \chi_n(y_0) |_{(z=z_R,y) \in \Gamma_R \& (z_0=z_R,y_0) \in \Gamma_R} dy dy_0 &= \\ \{ \delta_{kron}(n, m) \phi_n^-(z_0 = z_R) + S_{22}^{nm} \phi_n^+(z_0 = z_R) \} |_{z_0=z_R \in \Gamma_R} \end{aligned} \quad (A.124)$$

Mathematically, there are 4 different possibilities with respect to the nature of incident and reflected modes.

Case 1 : Both input and output modes are propagating $m \leq M_{prop}$ and $n \leq N_{prop}$

$$\begin{aligned} 2ik_z^{(m)} \frac{e^{-iz_R k_z^{(m)}}}{\sqrt{k_z^{(m)}}} \int_{y_0} \int_y \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) |_{(z=z_R,y) \in \Gamma_R \& (z_0=z_R,y_0) \in \Gamma_R} dy dy_0 &= \\ \delta_{kron}(n, m) \frac{e^{-iz_R k_z^{(n)}}}{\sqrt{k_z^{(n)}}} + S_{22}^{nm} \frac{e^{+iz_R k_z^{(n)}}}{\sqrt{k_z^{(n)}}} \end{aligned} \quad (A.125)$$

Case 2 : Input mode and output modes are evanescent $m > M_{prop}$ and $n > N_{prop}$

$$\begin{aligned} 2ik_z^{(m)} \frac{1}{\sqrt{|k_z^{(m)}|}} \int_{y_0} \int_y \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) |_{(z=z_R,y) \in \Gamma_R \& (z_0=z_R,y_0) \in \Gamma_R} dy dy_0 &= \\ \delta_{kron}(n, m) \frac{1}{\sqrt{|k_z^{(n)}|}} + S_{22}^{nm} \frac{1}{\sqrt{|k_z^{(n)}|}} \end{aligned} \quad (A.126)$$

Case 3 : Input modes are propagating and output modes are evanescent $m \leq M_{prop}$ and $n > N_{prop}$

$$\begin{aligned}
& 2ik_z^{(m)} \frac{e^{-iz_R k_z^{(m)}}}{\sqrt{k_z^{(m)}}} \int_{y_0} \int_y \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) |_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_L} dy dy_0 = \\
& \delta_{\text{kron}}(n, m) \frac{e^{-iz_R k_z^{(n)}}}{\sqrt{k_z^{(n)}}} + S_{22}^{nm} \frac{1}{\sqrt{|k_z^{(n)}|}}
\end{aligned} \tag{A.127}$$

But $\delta_{\text{kron}}(n, m) = 0$, if $m \leq M_{\text{prop}}$ and $n > N_{\text{prop}}$.

Case 4 : Input modes are evanescent and output modes are propagating $m > M_{\text{prop}}$ and $n \leq N_{\text{prop}}$

$$\begin{aligned}
& 2ik_z^{(m)} \frac{1}{\sqrt{|k_z^{(m)}|}} \int_{y_0} \int_y \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) |_{(z,y) \in \Gamma_L \& (z_0,y_0) \in \Gamma_L} dy dy_0 = \\
& \delta_{\text{kron}}(n, m) \frac{1}{\sqrt{|k_z^{(n)}|}} + S_{22}^{nm} \frac{e^{+iz_R k_z^{(n)}}}{\sqrt{k_z^{(n)}}}
\end{aligned} \tag{A.128}$$

But $\delta_{\text{kron}}(n, m) = 0$, if $m > M_{\text{prop}}$ and $n \leq N_{\text{prop}}$.

Solving S_{22} for cases 1, 2, 3 and 4 (using the information that for evanescent modes $\frac{k_z^{(m)}}{\sqrt{|k_z^{(m)}|}} = i\sqrt{|k_z^{(m)}|}$, is imaginary) are summarised in the Table 1.3.

A.11.4 Derivation for S_{12}

Let the wave incidence be from the right side of the disorder onto Γ_R . For estimating the transmission matrix S_{12} , need to take $(z_0, y_0) \in \Gamma_L$. Then the simplified boundary integral equation becomes,

$$\begin{aligned}
\sum_{m=1}^{M_{\text{total}}} 2ik_z^{(m)} \int E_m^{\text{inc}}(z, y) G(z, y, z_0, y_0) dy |_{(z,y) \in \Gamma_R \& (z_0,y_0) \in \Gamma_L} &= \sum_{n=1}^{N_{\text{total}}} E_n(z_0, y_0) |_{(z_0,y_0) \in \Gamma_L} \\
&= \sum_{n=1}^{N_{\text{total}}} \left\{ \sum_{m=1}^{M_{\text{total}}} c_m^+ S_{12}^{nm} \right\} \chi_n(y_0) \phi_n^-(z_0) |_{(z_0,y_0) \in \Gamma_L}
\end{aligned} \tag{A.129}$$

Performing the same set of operations as used for the derivation of S_{21} and setting $z = z_R$ and $z_0 = z_L$, the following is obtained

$$\begin{aligned}
& 2ik_z^{(m)} \phi_m^-(z = z_R) \int_y \int_{y_0} \chi_m(y) G(z = z_R, y, z_0 = z_L, y_0) \chi_n(y_0) dy dy_0 |_{(z=z_R,y) \in \Gamma_R \& (z_0=z_L,y_0) \in \Gamma_L} = \\
& S_{12}^{nm} \phi_n^-(z_0) |_{(z_0=z_L) \in \Gamma_L}
\end{aligned} \tag{A.130}$$

Mathematically, there are 4 different possibilities with respect to the nature of incident and transmitted modes.

Case 1 : Both input and output modes are propagating $m \leq M_{\text{prop}}$ and $n \leq N_{\text{prop}}$

$$2ik_z^{(m)} \frac{e^{-iz_R k_z^{(m)}}}{\sqrt{k_z^{(m)}}} \int_y \int_{y_0} \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) dy dy_0 |_{(z=z_R,y) \in \Gamma_R \& (z_0=z_L,y_0) \in \Gamma_L} = S_{12}^{nm} \frac{1}{\sqrt{k_z^{(n)}}} \tag{A.131}$$

Case 2 : Input mode and output modes are evanescent $m > M_{prop}$ and $n > N_{prop}$

$$2ik_z^{(m)} \frac{1}{\sqrt{|k_z^{(m)}|}} \int_y \int_{y_0} \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) dy dy_0 |_{(z=z_R, y) \in \Gamma_R \& (z_0=z_L, y_0) \in \Gamma_L} = S_{12}^{nm} \frac{1}{\sqrt{|k_z^{(n)}|}} \quad (\text{A.132})$$

Case 3 : Input modes are propagating and output modes are evanescent $m \leq M_{prop}$ and $n > N_{prop}$

$$2ik_z^{(m)} \frac{e^{-iz_R k_z^{(m)}}}{\sqrt{|k_z^{(m)}|}} \int_y \int_{y_0} \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) dy dy_0 |_{(z=z_R, y) \in \Gamma_R \& (z_0=z_L, y_0) \in \Gamma_L} = S_{12}^{nm} \frac{1}{\sqrt{|k_z^{(n)}|}} \quad (\text{A.133})$$

Case 4 : Input modes are evanescent and output modes are propagating $m > M_{prop}$ and $n \leq N_{prop}$

$$2ik_z^{(m)} \frac{1}{\sqrt{|k_z^{(m)}|}} \int_y \int_{y_0} \chi_m(y) G(z, y, z_0, y_0) \chi_n(y_0) dy dy_0 |_{(z, y) \in \Gamma_L \& (z_0, y_0) \in \Gamma_R} = \frac{S_{12}^{nm}}{\sqrt{|k_z^{(n)}|}} \quad (\text{A.134})$$

Solving S_{12} for cases 1, 2, 3 and 4 (using the information that for evanescent modes $\frac{k_z^{(m)}}{\sqrt{|k_z^{(m)}|}} = i\sqrt{|k_z^{(m)}|}$, is imaginary) are summarised in the Table 1.4.

A.12 Coherent mean-field attenuation and spatial correlation of the disorder

This section reviews how the attenuation of the coherent mean-field is affected by the spatial correlation of the disorder. Consider the Helmholtz equation

$$[\nabla^2 + k_0^2 \tilde{\epsilon}_r(z, y)] \psi(z, y) = 0 \quad (\text{A.135})$$

Let the fundamental distance measures z and y be expressed in terms of spatial correlation length l_c scaled by dimensionless scaling factor $\tilde{z}$ and $\tilde{y}$ such that $z = \tilde{z}l_c$ and $y = \tilde{y}l_c$. Then $\frac{\partial}{\partial z} = \frac{\partial \tilde{z}}{\partial z} \frac{\partial}{\partial \tilde{z}} = l_c \frac{\partial}{\partial \tilde{z}}$. Therefore, $\frac{\partial}{\partial z} = \frac{1}{l_c} \frac{\partial}{\partial \tilde{z}}$ and $\frac{\partial^2}{\partial z^2} = \frac{1}{l_c^2} \frac{\partial^2}{\partial \tilde{z}^2}$. Similarly, for y as well. Therefore Helmholtz equation can be non-dimensionalised[30] as the following

$$\left[\frac{1}{l_c^2} \tilde{\nabla}^2 + k_0^2 \tilde{\epsilon}_r(\tilde{z}, \tilde{y}) \right] \psi(\tilde{z}, \tilde{y}) = 0 \implies [\tilde{\nabla}^2 + (k_0 l_c)^2 \tilde{\epsilon}_r(\tilde{z}, \tilde{y})] \psi(\tilde{z}, \tilde{y}) = 0 \quad (\text{A.136})$$

Disorder dielectric constant $\tilde{\epsilon}_r(\tilde{z}, \tilde{y})$ can be written as a spatial perturbation around the reference value as $\tilde{\epsilon}_r(\tilde{z}, \tilde{y}) = \tilde{\epsilon}_r^{ref} + \delta \tilde{\epsilon}_r(\tilde{z}, \tilde{y})$. Substituting the disorder perturbation in the Helmholtz equation and taking $k_0^2 \tilde{\epsilon}_r$ as k_{ref}^2

$$[\tilde{\nabla}^2 + (k_{ref} l_c)^2] \psi(\tilde{z}, \tilde{y}) = \underbrace{-(k_0 l_c)^2 \delta \tilde{\epsilon}_r(\tilde{z}, \tilde{y})}_{V(\tilde{z}, \tilde{y})} \psi(\tilde{z}, \tilde{y}) \quad (\text{A.137})$$

where $V(\tilde{z}, \tilde{y})$ is the scattering potential of the correlated disorder. According to Section 1.4, perturbed Green's function $G(\tilde{r}, \tilde{r}_0)$ for this disorder is given by Dyson's equation as given below

$$G(\tilde{r}, \tilde{r}_0) = G_0(\tilde{r}, \tilde{r}_0) + \int_{\tilde{r}_1} G_0(\tilde{r}, \tilde{r}_1) V(\tilde{r}_1) G(\tilde{r}_1, \tilde{r}_0) d\tilde{r}_1 \quad (\text{A.138})$$

where $G_0(\tilde{r}, \tilde{r}_0)$ is the Green's function without any disorder with a wavevector magnitude of k_{ref} . As $G(\tilde{r}, \tilde{r}_0)$ appears both on the *L.H.S* and *R.H.S* of the above equation, the Green's function has an iterative structure. Hence Dyson's equation can be expanded as a perturbation series. Hence, use the following expressions

$$G(\tilde{r}_1, \tilde{r}_0) = G_0(\tilde{r}_1, \tilde{r}_0) + \int_{\tilde{r}_2} G_0(\tilde{r}_1, \tilde{r}_2) V(\tilde{r}_2) G(\tilde{r}_2, \tilde{r}_0) d\tilde{r}_2 \quad (\text{A.139})$$

$$G(\tilde{r}_2, \tilde{r}_0) = G_0(\tilde{r}_2, \tilde{r}_0) + \int_{\tilde{r}_3} G_0(\tilde{r}_2, \tilde{r}_3) V(\tilde{r}_3) G(\tilde{r}_3, \tilde{r}_0) d\tilde{r}_3 \quad (\text{A.140})$$

$$G(\tilde{r}_3, \tilde{r}_0) = G_0(\tilde{r}_3, \tilde{r}_0) + \int_{\tilde{r}_4} G_0(\tilde{r}_3, \tilde{r}_4) V(\tilde{r}_4) G(\tilde{r}_4, \tilde{r}_0) d\tilde{r}_4 \quad (\text{A.141})$$

$$G(\tilde{r}_4, \tilde{r}_0) = G_0(\tilde{r}_4, \tilde{r}_0) + \int_{\tilde{r}_5} G_0(\tilde{r}_4, \tilde{r}_5) V(\tilde{r}_5) G(\tilde{r}_5, \tilde{r}_0) d\tilde{r}_5 \quad (\text{A.142})$$

to substitute in the main Dyson's equation (equation A.138) to obtain the following perturbation series indicative of the analytic structure of multiple scattering

$$\begin{aligned} G(\tilde{r}, \tilde{r}_0) &= \overbrace{G_0(\tilde{r}, \tilde{r}_0)}^{\tilde{r}_0 \rightarrow \tilde{r}} + \int_{\tilde{r}_1} \overbrace{G_0(\tilde{r}, \tilde{r}_1) V(\tilde{r}_1) G_0(\tilde{r}_1, \tilde{r}_0)}^{\tilde{r}_0 \rightarrow \bullet \rightarrow \tilde{r}} d\tilde{r}_1 + \\ &\int_{\tilde{r}_1} \int_{\tilde{r}_2} \overbrace{G_0(\tilde{r}, \tilde{r}_1) V(\tilde{r}_1) G_0(\tilde{r}_1, \tilde{r}_2) V(\tilde{r}_2) G_0(\tilde{r}_2, \tilde{r}_0)}^{\tilde{r}_0 \rightarrow \bullet \rightarrow \bullet \rightarrow r} d\tilde{r}_2 d\tilde{r}_1 + \\ &\int_{\tilde{r}_1} \int_{\tilde{r}_2} \int_{\tilde{r}_3} \overbrace{G_0(\tilde{r}, \tilde{r}_1) V(\tilde{r}_1) G_0(\tilde{r}_1, \tilde{r}_2) V(\tilde{r}_2) G_0(\tilde{r}_2, \tilde{r}_3) V(\tilde{r}_3) G_0(\tilde{r}_3, \tilde{r}_0)}^{\tilde{r}_0 \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow r} d\tilde{r}_3 d\tilde{r}_2 d\tilde{r}_1 + \\ &\int_{\tilde{r}_1} \int_{\tilde{r}_2} \int_{\tilde{r}_3} \int_{\tilde{r}_4} \overbrace{G_0(\tilde{r}, \tilde{r}_1) V(\tilde{r}_1) G_0(\tilde{r}_1, \tilde{r}_2) V(\tilde{r}_2) G_0(\tilde{r}_2, \tilde{r}_3) V(\tilde{r}_3) G_0(\tilde{r}_3, \tilde{r}_4) V(\tilde{r}_4) G_0(\tilde{r}_4, \tilde{r}_0)}^{\tilde{r}_0 \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow r} d\tilde{r}_4 d\tilde{r}_3 d\tilde{r}_2 d\tilde{r}_1 + \dots \end{aligned} \quad (\text{A.144})$$

Next, ensemble averaged (over many realisations of disorder) coherent mean-field component of the Green's function is estimated. Ensemble averaging acts only on the random variables such as $V(r_i)$

and not on deterministic terms such as $G_0(r_j, r_i)$. Hence,

$$\langle G(\tilde{r}, \tilde{r}_0) \rangle = \overbrace{G_0(\tilde{r}, \tilde{r}_0)}^{\tilde{r}_0 \rightarrow \tilde{r}} + \int_{\tilde{r}_1} \overbrace{G_0(\tilde{r}, \tilde{r}_1) \langle V(\tilde{r}_1) \rangle G_0(\tilde{r}_1, \tilde{r}_0)}^{\tilde{r}_0 \rightarrow \bullet \xrightarrow{\tilde{r}_1} \tilde{r}} d\tilde{r}_1 + \quad (\text{A.145})$$

$$\begin{aligned} & \int_{\tilde{r}_1} \int_{\tilde{r}_2} \overbrace{G_0(\tilde{r}, \tilde{r}_1) G_0(\tilde{r}_1, \tilde{r}_2) \langle V(\tilde{r}_1) V(\tilde{r}_2) \rangle G_0(\tilde{r}_2, \tilde{r}_0)}^{\tilde{r}_0 \rightarrow \bullet \xrightarrow{\tilde{r}_2} \bullet \xrightarrow{\tilde{r}_1} r} d\tilde{r}_2 d\tilde{r}_1 + \\ & \int_{\tilde{r}_1} \int_{\tilde{r}_2} \int_{\tilde{r}_3} \overbrace{G_0(\tilde{r}, \tilde{r}_1) G_0(\tilde{r}_1, \tilde{r}_2) G_0(\tilde{r}_2, \tilde{r}_3) \langle V(\tilde{r}_1) V(\tilde{r}_2) V(\tilde{r}_3) \rangle G_0(\tilde{r}_3, \tilde{r}_0)}^{\tilde{r}_0 \rightarrow \bullet \xrightarrow{\tilde{r}_3} \bullet \xrightarrow{\tilde{r}_2} \bullet \xrightarrow{\tilde{r}_1} r} d\tilde{r}_3 d\tilde{r}_2 d\tilde{r}_1 + \\ & \int_{\tilde{r}_1} \int_{\tilde{r}_2} \int_{\tilde{r}_3} \int_{\tilde{r}_4} \overbrace{G_0(\tilde{r}, \tilde{r}_1) G_0(\tilde{r}_1, \tilde{r}_2) G_0(\tilde{r}_2, \tilde{r}_3) G_0(\tilde{r}_3, \tilde{r}_4) \langle V(\tilde{r}_1) V(\tilde{r}_2) V(\tilde{r}_3) V(\tilde{r}_4) \rangle G_0(\tilde{r}_4, \tilde{r}_0)}^{\tilde{r}_0 \rightarrow \bullet \xrightarrow{\tilde{r}_4} \bullet \xrightarrow{\tilde{r}_3} \bullet \xrightarrow{\tilde{r}_2} \bullet \xrightarrow{\tilde{r}_1} r} d\tilde{r}_4 d\tilde{r}_3 d\tilde{r}_2 d\tilde{r}_1 + \dots \end{aligned} \quad (\text{A.146})$$

Hence, spatial correlation functions $\langle V(\tilde{r}_1) \rangle$, $\langle V(\tilde{r}_1) V(\tilde{r}_2) \rangle$, $\langle V(\tilde{r}_1) V(\tilde{r}_2) V(\tilde{r}_3) \rangle$, etc... determines the coherent mean-field component of the Green's function upon ensemble averaging. As $\langle V(\tilde{r}_1) \rangle$ is a zero mean field, $\langle V(\tilde{r}_1) \rangle = 0$. Fortunately due to the properties of Gaussian random fields (refer equation 1.128 of [110]), odd number of terms inside the ensemble averaging makes it zero. As an example, $\langle V(\tilde{r}_1) V(\tilde{r}_2) V(\tilde{r}_3) \rangle = 0$. In addition to that, any even number of terms inside a Gaussian correlation function can be factorised into a combination of two-point correlation functions. As an example, $\langle V(\tilde{r}_1) V(\tilde{r}_2) V(\tilde{r}_3) V(\tilde{r}_4) \rangle$ can be written as

$$\begin{aligned} \langle V(\tilde{r}_1) V(\tilde{r}_2) V(\tilde{r}_3) V(\tilde{r}_4) \rangle &= \langle V(\tilde{r}_1) V(\tilde{r}_2) \rangle \langle V(\tilde{r}_3) V(\tilde{r}_4) \rangle + \\ & \langle V(\tilde{r}_1) V(\tilde{r}_3) \rangle \langle V(\tilde{r}_2) V(\tilde{r}_4) \rangle + \\ & \langle V(\tilde{r}_1) V(\tilde{r}_4) \rangle \langle V(\tilde{r}_2) V(\tilde{r}_3) \rangle \end{aligned} \quad (\text{A.147})$$

This leads to a systematic study of perturbation series for multiple scattering involving two-point Gaussian correlation functions $\langle V(\tilde{r}_i) V(\tilde{r}_j) \rangle$. For detailed analysis on the subject of perturbation theory for multiple scattering, refer to [30, 66, 67, 111]. Until now, the only assumption taken is that the disorder spatial correlation function is Gaussian. To proceed analytically from here, approximations have to be taken on the perturbation series to make physical interpretation out of that. Simplest approximation to the perturbation series given in equation A.146 is the Bourret approximation, leading to the formulation of the following iterative mean-field equation.

$$\langle G(\tilde{r}, \tilde{r}_0) \rangle = G_0(\tilde{r}, \tilde{r}_0) + \int_{\tilde{r}_1} \int_{\tilde{r}_2} G_0(\tilde{r}, \tilde{r}_1) G_0(\tilde{r}_1, \tilde{r}_2) \langle V(\tilde{r}_1) V(\tilde{r}_2) \rangle \langle G(\tilde{r}_2, \tilde{r}_0) \rangle d\tilde{r}_2 d\tilde{r}_1 \quad (\text{A.148})$$

Applying $[\tilde{\nabla}^2 + (k_{ref} l_c)^2]$ on the L.H.S and R.H.S of the above given equation,

$$\begin{aligned} [\tilde{\nabla}^2 + (k_{ref} l_c)^2] \langle G(\tilde{r}, \tilde{r}_0) \rangle &= [\tilde{\nabla}^2 + (k_{ref} l_c)^2] G_0(\tilde{r}, \tilde{r}_0) + \\ & \int_{\tilde{r}_1} \int_{\tilde{r}_2} [\tilde{\nabla}^2 + (k_{ref} l_c)^2] G_0(\tilde{r}, \tilde{r}_1) G_0(\tilde{r}_1, \tilde{r}_2) \langle V(\tilde{r}_1) V(\tilde{r}_2) \rangle \langle G(\tilde{r}_2, \tilde{r}_0) \rangle d\tilde{r}_2 d\tilde{r}_1 \end{aligned} \quad (\text{A.149})$$

On simplification,

$$\begin{aligned} [\tilde{\nabla}^2 + (k_{ref} l_c)^2] \langle G(\tilde{r}, \tilde{r}_0) \rangle &= \delta(\tilde{r}, \tilde{r}_0) + \\ & \int_{\tilde{r}_1} \int_{\tilde{r}_2} \delta(\tilde{r}, \tilde{r}_1) G_0(\tilde{r}_1, \tilde{r}_2) \langle V(\tilde{r}_1) V(\tilde{r}_2) \rangle \langle G(\tilde{r}_2, \tilde{r}_0) \rangle d\tilde{r}_2 d\tilde{r}_1 \end{aligned} \quad (\text{A.150})$$

The Bourret equation can again be simplified and re-arranged to obtain

$$[\tilde{\nabla}^2 + (k_{ref}l_c)^2] \langle G(\tilde{r}, \tilde{r}_0) \rangle - \int_{\tilde{r}_1} G_0(\tilde{r}, \tilde{r}_1) \langle V(\tilde{r})V(\tilde{r}_1) \rangle \langle G(\tilde{r}_1, \tilde{r}_0) \rangle d\tilde{r}_1 = \delta(\tilde{r}, \tilde{r}_0) \quad (A.151)$$

As $V(\tilde{z}, \tilde{y}) = -(k_0l_c)^2 \delta\tilde{\epsilon}_r(\tilde{z}, \tilde{y})$, the above given equation can be re-written as

$$[\tilde{\nabla}^2 + (k_{ref}l_c)^2] \langle G(\tilde{r}, \tilde{r}_0) \rangle - (k_0l_c)^2 \int_{\tilde{r}_1} G_0(\tilde{r}, \tilde{r}_1) \{ (k_0l_c)^2 \langle \delta\tilde{\epsilon}_r(\tilde{r})\delta\tilde{\epsilon}_r(\tilde{r}_1) \rangle \} \langle G(\tilde{r}_1, \tilde{r}_0) \rangle d\tilde{r}_1 = \delta(\tilde{r}, \tilde{r}_0) \quad (A.152)$$

The above given equation is the Bourret equation for the coherent mean-field, where the mean-field propagates in an effective attenuating medium. One may notice that the equation is parametrised by the term $(k_0l_c)^2 \langle \delta\tilde{\epsilon}_r(\tilde{r})\delta\tilde{\epsilon}_r(\tilde{r}_1) \rangle$, maximum value of which is referred to as the generalised Reynolds number R_e . In this thesis, as all the lengths are made dimensionless using k_{ref} , the generalised Reynolds number is redefined in terms of k_{ref} for consistency. Therefore $R_e = (k_{ref}l_c)^2 var_{disorder}$

A.13 Steady-state analytical solution to the diffusion equation for the slab geometry

The steady-state diffusion approximation of the diffuson $P_d(r, r_0)$ is obtained by solving the following Green's function problem in the spatial Fourier domain

$$-D_e \nabla^2 P_d(r, r_0) = \delta(r - r_0) \quad (A.153)$$

where $D_e = cl^*/d$ is the diffusion constant, d is the dimensionality of the problem ($d = 2$ for 2D and $d = 3$ for 3D), l^* is the transport mean-free path and r_0 , the source position. In this section, $P_d(r, r_0)$ is solved for a 2D problem of an infinitely extending slab along the transverse dimension (along y) and finite sized (of size L) along the longitudinal dimension (along z). Solution for the 3D problem, follows the same logic. Two kinds of z boundary conditions exist at $z = 0$ and $z = L$. Simplest of those two boundary conditions is the absorbing boundary condition where $P_d(y, z = 0) = P_d(y, z = L) = 0$ is set at the two ends of the slab. A better and realistic boundary condition is the extrapolated/partially absorbing/Robin boundary conditions (known by different names). $P_d(r, r_0)$ is solved using both the boundary conditions in the subsections. To proceed further, $P_d(r, r_0)$ is assumed to have translational invariance with respect to y so that $P_d(z, z_0, y, y_0)$ depends only on $y - y_0$. Hence $P_d(z, z_0, y, y_0) = P_d(z, z_0, y - y_0) = P_d(z, z_0, \rho)$ where $\rho = y - y_0$ is a new variable denoting the relative displacement with respect to the source y_0 location. Then diffusion equation (equation A.153) in 2D takes the form

$$-D_e \left\{ \frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial \rho^2} \right\} P_d(z, z_0, \rho) = \delta(\rho)\delta(z - z_0) \quad (A.154)$$

whose spatial Fourier transform, transforming $\rho \rightarrow q$ has the form

$$\left\{ \frac{\partial^2}{\partial z^2} - q^2 \right\} P_d(z, z_0, q) = \frac{-1}{D_e} \delta(z - z_0) \quad (A.155)$$

This 1D Green's function problem for the diffusion equation is solved using the very similar ideas given in Section A.3.1 for the 1D wave equation Green's function problem. As there is a $\delta(z - z_0)$ on the R.H.S, the solution $P_d(z, z_0, q)$ has to be split for two regions, $z > z_0$ and $z < z_0$.

$$P_d(z, z_0, q) = \begin{cases} P_d^+(z, z_0, q) & \text{if } z \geq z_0 \\ P_d^-(z, z_0, q) & \text{if } z < z_0 \end{cases} \quad (A.156)$$

As discussed in Section A.3.1, the Dirac-delta function in equation A.155, implies that there is a discontinuity for the first order derivative as given below

$$\frac{\partial}{\partial z} P_d^+(z, z_0, q)|_{z=z_0} - \frac{\partial}{\partial z} P_d^-(z, z_0, q)|_{z=z_0} = \frac{-1}{D_e} \quad (\text{A.157})$$

In addition to that, due to continuity of $P_d(z, z_0, q)$ at $z = z_0$

$$P_d^+(z = z_0, z_0, q) = P_d^-(z = z_0, z_0, q) \quad (\text{A.158})$$

Without the source, the Fourier transformed diffusion equation

$$\left\{ \frac{\partial^2}{\partial z^2} - q^2 \right\} P_d(z, q) = 0 \quad (\text{A.159})$$

has the following homogeneous general solution

$$P_d(z, q) = A \sinh(qz) + B \cosh(qz) \quad (\text{A.160})$$

Hence, equation A.156 could be written in the following form

$$P_d(z, z_0, q) = \begin{cases} P_d^+(z, z_0, q) = c_1 \sinh(q(z - z_0)) + c_2 \cosh(q(z - z_0)) & \text{if } z \geq z_0 \\ P_d^-(z, z_0, q) = c_3 \sinh(-q(z - z_0)) + c_4 \cosh(-q(z - z_0)) & \text{if } z < z_0 \end{cases} \quad (\text{A.161})$$

For solving the 4 unknowns c_1, c_2, c_3 and c_4 , two z boundary conditions have to be introduced, in addition to equations A.155 and A.158. Firstly, the Robin boundary conditions are discussed in the following section.

A.13.1 Solving the diffusion equation using extrapolated/partially absorbing/Robin boundary conditions

Fourier transformed Robin boundary conditions at $z = 0$ and $z = L$ are given as the following

$$P_d^+(z, z_0, q)|_{z=L} + z_e l^* \frac{\partial}{\partial z} P_d^+(z, z_0, q)|_{z=L} = 0 \quad (\text{A.162})$$

$$P_d^-(z, z_0, q)|_{z=0} - z_e l^* \frac{\partial}{\partial z} P_d^-(z, z_0, q)|_{z=0} = 0 \quad (\text{A.163})$$

where z_e is the dimensionless extrapolation length ratio such that $z_e l^*$ is the length of the extrapolated boundary from the surface. For a refractive index matched sample $z_e = 2/3$ for 3D and $z_e = \pi/4$ for 2D. Substituting equation A.161 in the Robin boundary conditions, the following set of equations are obtained.

$$c_1 \{ \sinh(q(L - z_0)) + l^* z_e q \cosh(q(L - z_0)) \} + c_2 \{ \cosh(q(L - z_0)) + l^* q z_e \sinh(q(L - z_0)) \} = 0 \quad (\text{A.164})$$

$$c_3 \{ q l^* z_e \cosh(q z_0) + \sinh(q z_0) \} + c_4 \{ q l^* z_e \sinh(q z_0) + \cosh(q z_0) \} = 0 \quad (\text{A.165})$$

Substituting equation A.161 in equation A.157 yields

$$c_1 q + c_3 q = \frac{-1}{D_e} \quad (\text{A.166})$$

Substituting equation A.161 in equation A.158 yields

$$c_2 - c_4 = 0 \quad (\text{A.167})$$

Using Mathematica, four unknowns c_1, c_2, c_3 and c_4 are solved from the previously given four equations to obtain

$$c_1 = -\frac{(ql^*z_e \cosh(qz_0) + \sinh(qz_0))(ql^*z_e \sinh(q(L-z_0)) + \cosh(q(L-z_0)))}{qD_e \left(\sinh(Lq) \left(q^2 l^{*2} z_e^2 + 1 \right) + 2ql^*z_e \cosh(Lq) \right)} \quad (\text{A.168})$$

$$c_2 = \frac{(ql^*z_e \cosh(qz_0) + \sinh(qz_0))(ql^*z_e \cosh(q(L-z_0)) + \sinh(q(L-z_0)))}{qD_e \left(\sinh(Lq) \left(q^2 l^{*2} z_e^2 + 1 \right) + 2ql^*z_e \cosh(Lq) \right)} \quad (\text{A.169})$$

$$c_3 = -\frac{(ql^*z_e \sinh(qz_0) + \cosh(qz_0))(ql^*z_e \cosh(q(L-z_0)) + \sinh(q(L-z_0)))}{qD_e \left(\sinh(Lq) \left(q^2 l^{*2} z_e^2 + 1 \right) + 2ql^*z_e \cosh(Lq) \right)} \quad (\text{A.170})$$

$$c_4 = \frac{(ql^*z_e \cosh(qz_0) + \sinh(qz_0))(ql^*z_e \cosh(q(L-z_0)) + \sinh(q(L-z_0)))}{qD_e \left(\sinh(Lq) \left(q^2 l^{*2} z_e^2 + 1 \right) + 2ql^*z_e \cosh(Lq) \right)} \quad (\text{A.171})$$

Substituting c_1 and c_2 in A.161 for $P_d^+(z, z_0, q)$ and simplifying using Mathematica

$$P_d^+(z, z_0, q) = \frac{(ql^*z_e \cosh(qz_0) + \sinh(qz_0))(ql^*z_e \cosh(q(L-z)) + \sinh(q(L-z)))}{qD_e \left(\sinh(Lq) \left(q^2 l^{*2} z_e^2 + 1 \right) + 2ql^*z_e \cosh(Lq) \right)} \quad (\text{A.172})$$

y integrated $P_d^+(z, z_0, q)$ at various z values is obtained by the Fourier technique of taking the limit at $q = 0$ as the following

$$\int_{-\infty}^{+\infty} P_d^+(z, z_0, y) dy = \lim_{q \rightarrow 0} P_d^+(z, z_0, q) = \frac{(l^*z_e + z_0)(l^*z_e + L - z)}{D_e(2l^*z_e + L)} \quad (\text{A.173})$$

which is indeed the solution to a 1D diffusion equation. Total transmission can be estimated as the following

$$T = -D_e \frac{\partial}{\partial z} \left\{ \int_{-\infty}^{+\infty} P_d^+(z, z_0, y) dy \right\} \Big|_{z=L} = \frac{l^*z_e + z_0}{L + 2l^*z_e} = \frac{z_e + \frac{z_0}{l^*}}{\frac{L}{l^*} + 2z_e} \quad (\text{A.174})$$

which is the well known expression for total transmission reported in [70, 77] for $z_0 = l^*$. If $L/l^* \gg 1$ and the source injection point z_0 is taken as l^* , then the total transmission can be approximated as

$$T = \frac{z_e + \frac{z_0}{l^*}}{\frac{L}{l^*} + 2z_e} \approx \frac{z_e + 1}{\frac{L}{l^*}} = \begin{cases} \frac{5}{3} \frac{l^*}{L} \text{ where } z_e = 2/3 \text{ for } 3D \text{ such that } L/l^* \gg 1 \\ (1 + \frac{\pi}{4}) \frac{l^*}{L} \text{ where } z_e = \pi/4 \text{ for } 2D \text{ such that } L/l^* \gg 1 \end{cases} \quad (\text{A.175})$$

Similarly, substituting c_3 and c_4 in equation A.161 for $P_d^-(z, z_0, q)$ and simplifying using Mathematica

$$P_d^-(z, z_0, q) = \frac{(ql^*z_e \cosh(qz) + \sinh(qz))(ql^*z_e \cosh(q(L-z_0)) + \sinh(q(L-z_0)))}{qD_e \left(\sinh(Lq) \left(q^2 l^{*2} z_e^2 + 1 \right) + 2ql^*z_e \cosh(Lq) \right)} \quad (\text{A.176})$$

y integrated $P_d^-(z, z_0, q)$ at various z values is obtained by the same Fourier technique of taking the limit at $q = 0$ as the following

$$\int_{-\infty}^{+\infty} P_d^-(z, z_0, y) dy = \lim_{q \rightarrow 0} P_d^-(z, z_0, q) = \frac{(l^*z_e + z)(l^*z_e + L - z_0)}{D_e(2l^*z_e + L)} \quad (\text{A.177})$$

Total reflection can be estimated as the following

$$R = +D_e \frac{\partial}{\partial z} \left\{ \int_{-\infty}^{+\infty} P_d^-(z, z_0, y) dy \right\} \Big|_{z=0} = \frac{l^*z_e + L - z_0}{L + 2l^*z_e} = \frac{z_e + \frac{L}{l^*} - \frac{z_0}{l^*}}{\frac{L}{l^*} + 2z_e} \quad (\text{A.178})$$

Using the expressions for R and T , flux conservation can be verified as $R + T = 1$.

A.14 Derivation for the FDTD Absorbing Boundary Condition (analytical) at $z = 0$ and $z = z_{end}$

Refer Figure 3.4 given in the Chapter 2 for the following derivation. ABC is incorporated at $z = 0$ and $z = z_{end}$ as shown in the figure, at half-way between interior nodes and boundary nodes. Hence, special care has to be taken to define derivatives at $i = \frac{1}{2}$ and $i = N_z + \frac{1}{2}$. (All other definitions of derivative operators given in Chapter 2 were evaluated at the interior grid nodes and not at half-distances from the grid nodes). The goal is to obtain a time-stepping equation for the boundary node fields $E_{0,j}^{n+1}$ and $E_{N_z+1,j}^{n+1}$ based on the equations 3.7 and 3.8, respectively.

A.14.1 FDTD formulation of the ABC at $z = 0$

$$\frac{\partial^2 E(r, t)}{\partial z \partial t} - \frac{p_0}{c_{\text{ref}}} \frac{\partial^2 E(r, t)}{\partial t^2} + p_2 c_{\text{ref}} \frac{\partial^2 E(r, t)}{\partial y^2} = 0 \quad (\text{A.179})$$

L.H.S of the above given equation is split into three terms as given below

$$\begin{aligned} \text{Term 1 : } \frac{\partial^2 E(r, t)}{\partial z \partial t} \Big|_{z=0, y, n} &= \frac{\partial}{\partial z} \frac{\partial}{\partial t} E(r, t) \Big|_{z=0, y, n} = \frac{\partial}{\partial z} \left(\frac{E_{i,j}^{n+1} - E_{i,j}^{n-1}}{2\Delta_t} \right) \Big|_{z=0, y, n} = \frac{\partial}{\partial z} \left(\frac{E_{i,j}^{n+1} - E_{i,j}^{n-1}}{2\Delta_t} \right) \Big|_{i=\frac{1}{2}, j, n} \\ &= \frac{1}{2\Delta_t} \left\{ \frac{E_{1,j}^{n+1} - E_{0,j}^{n+1}}{\Delta_z} - \frac{E_{1,j}^{n-1} - E_{0,j}^{n-1}}{\Delta_z} \right\} = \frac{1}{2\Delta_t \Delta_z} \left\{ \left(E_{1,j}^{n+1} - E_{0,j}^{n+1} \right) - \left(E_{1,j}^{n-1} - E_{0,j}^{n-1} \right) \right\} \end{aligned} \quad (\text{A.180})$$

$$\begin{aligned} \text{Term 2 : } -\frac{p_0}{c_{\text{ref}}} \frac{\partial^2 E(r, t)}{\partial t^2} \Big|_{z=0, j, n} &= -\frac{p_0}{c_{\text{ref}}} \frac{\partial^2 E(r, t)}{\partial t^2} \Big|_{i=\frac{1}{2}, j, n} = -\frac{p_0}{c_{\text{ref}}} \frac{1}{2} \left\{ \frac{\partial^2 E(r, t)}{\partial t^2} \Big|_{i=0, j, n} + \frac{\partial^2 E(r, t)}{\partial t^2} \Big|_{i=1, j, n} \right\} \\ &= -\frac{p_0}{2c_{\text{ref}}} \left(\frac{E_{0,j}^{n-1} + E_{0,j}^{n+1} - 2E_{0,j}^n}{\Delta_t^2} + \frac{E_{1,j}^{n-1} + E_{1,j}^{n+1} - 2E_{1,j}^n}{\Delta_t^2} \right) \\ &= -\frac{p_0}{2c_{\text{ref}} \Delta_t^2} \left\{ \left(E_{0,j}^{n-1} + E_{0,j}^{n+1} - 2E_{0,j}^n \right) + \left(E_{1,j}^{n-1} + E_{1,j}^{n+1} - 2E_{1,j}^n \right) \right\} \end{aligned} \quad (\text{A.181})$$

$$\begin{aligned} \text{Term 3 : } p_2 c_{\text{ref}} \frac{\partial^2 E(r, t)}{\partial y^2} \Big|_{z=0, y, n} &= p_2 c_{\text{ref}} \frac{\partial^2 E(r, t)}{\partial y^2} \Big|_{i=\frac{1}{2}, j, n} = p_2 c_{\text{ref}} \frac{1}{2} \left\{ \frac{\partial^2 E(r, t)}{\partial y^2} \Big|_{i=0, j, n} + \frac{\partial^2 E(r, t)}{\partial y^2} \Big|_{i=1, j, n} \right\} \\ &= \frac{1}{2} p_2 c_{\text{ref}} \left\{ \frac{E_{0,j-1}^n + E_{0,j+1}^n - 2E_{0,j}^n}{\Delta_y^2} + \frac{E_{1,j-1}^n + E_{1,j+1}^n - 2E_{1,j}^n}{\Delta_y^2} \right\} \\ &= \left(\frac{p_2 c_{\text{ref}}}{2\Delta_y^2} \right) \left\{ \left(E_{0,j-1}^n + E_{0,j+1}^n - 2E_{0,j}^n \right) + \left(E_{1,j-1}^n + E_{1,j+1}^n - 2E_{1,j}^n \right) \right\} \end{aligned} \quad (\text{A.182})$$

Equation A.179, is then given by $\text{Term 1} + \text{Term 2} + \text{Term 3} = 0$, as the following

$$\begin{aligned} &\frac{1}{2\Delta_t \Delta_z} \left\{ \left(E_{1,j}^{n+1} - E_{0,j}^{n+1} \right) - \left(E_{1,j}^{n-1} - E_{0,j}^{n-1} \right) \right\} - \frac{p_0}{2c_{\text{ref}} \Delta_t^2} \left\{ \left(E_{0,j}^{n-1} + E_{0,j}^{n+1} - 2E_{0,j}^n \right) + \left(E_{1,j}^{n-1} + E_{1,j}^{n+1} - 2E_{1,j}^n \right) \right\} + \\ &\frac{p_2 c_{\text{ref}}}{2\Delta_y^2} \left\{ \left(E_{0,j-1}^n + E_{0,j+1}^n - 2E_{0,j}^n \right) + \left(E_{1,j-1}^n + E_{1,j+1}^n - 2E_{1,j}^n \right) \right\} = 0 \end{aligned} \quad (\text{A.183})$$

Collecting the coefficients of $E_{0,j}^{n+1}$,

$$E_{0,j}^{n+1} \left(\frac{p_0}{2c_{\text{ref}}\Delta_t^2} + \frac{1}{2\Delta_t\Delta_z} \right) = \frac{1}{2\Delta_t\Delta_z} \left(E_{1,j}^{n+1} - (E_{1,j}^{n-1} - E_{0,j}^{n-1}) \right) - \frac{p_0}{2c_{\text{ref}}\Delta_t^2} \left((E_{0,j}^{n-1} - 2E_{0,j}^n) + (E_{1,j}^{n-1} + E_{1,j}^{n+1} - 2E_{1,j}^n) \right) \\ + \frac{p_2c_{\text{ref}}}{2\Delta_y^2} \left((E_{0,j-1}^n + E_{0,j+1}^n - 2E_{0,j}^n) + (E_{1,j-1}^n + E_{1,j+1}^n - 2E_{1,j}^n) \right) \quad (\text{A.184})$$

Re-arranging the terms for further simplification,

$$E_{0,j}^{n+1} \left(\frac{p_0}{2c_{\text{ref}}\Delta_t^2} + \frac{1}{2\Delta_t\Delta_z} \right) = - \left[\frac{p_0}{2c_{\text{ref}}\Delta_t^2} + \frac{1}{2\Delta_t\Delta_z} \right] E_{1,j}^{n-1} + \left[\frac{1}{2\Delta_t\Delta_z} - \frac{p_0}{2c_{\text{ref}}\Delta_t^2} \right] (E_{0,j}^{n-1} + E_{1,j}^{n+1}) + \\ \frac{p_0(E_{0,j}^n + E_{1,j}^n)}{c_{\text{ref}}\Delta_t^2} + \frac{p_2c_{\text{ref}}}{2\Delta_y^2} \left((E_{0,j-1}^n + E_{0,j+1}^n - 2E_{0,j}^n) + (E_{1,j-1}^n + E_{1,j+1}^n - 2E_{1,j}^n) \right) \quad (\text{A.185})$$

Upon simplifying to obtain $E_{0,j}^{n+1}$

$$E_{0,j}^{n+1} = -E_{1,j}^{n-1} + \frac{c_{\text{ref}}\Delta_t - p_0\Delta_z}{c_{\text{ref}}\Delta_t + p_0\Delta_z} (E_{0,j}^{n-1} + E_{1,j}^{n+1}) + \frac{2p_0\Delta_z}{c_{\text{ref}}\Delta_t + p_0\Delta_z} (E_{0,j}^n + E_{1,j}^n) + \\ \frac{p_2c_{\text{ref}}^2\Delta_t^2\Delta_z}{\Delta_y^2(c_{\text{ref}}\Delta_t + p_0\Delta_z)} \left\{ (E_{0,j-1}^n + E_{0,j+1}^n - 2E_{0,j}^n) + (E_{1,j-1}^n + E_{1,j+1}^n - 2E_{1,j}^n) \right\} \quad (\text{A.186})$$

A.14.2 FDTD formulation of the ABC at $z = z_{\text{end}}$

At $z = z_{\text{end}}$ or at $i = (N_z + \frac{1}{2})$

$$\frac{\partial^2 E(r, t)}{\partial z \partial t} + \frac{p_0}{c_{\text{ref}}} \frac{\partial^2 E(r, t)}{\partial t^2} - p_2c_{\text{ref}} \frac{\partial^2 E(r, t)}{\partial y^2} = 0 \quad (\text{A.187})$$

Following the same analysis given in the previous subsection for $z = 0$, time stepping equation can be obtained for the boundary node at $N_z + 1$ (shown in Figure 3.4 of Chapter 2). For brevity, the steps taken, which are very similar to previous subsection for $z = 0$, are not repeated once again. Instead the final result is presented below

$$E_{N_z+1,j}^{n+1} = -E_{N_z,j}^{n-1} + \frac{c_{\text{ref}}\Delta_t - p_0\Delta_z}{c_{\text{ref}}\Delta_t + p_0\Delta_z} (E_{N_z+1,j}^{n-1} + E_{N_z,j}^{n+1}) + \frac{2p_0\Delta_z}{c_{\text{ref}}\Delta_t + p_0\Delta_z} (E_{N_z+1,j}^n + E_{N_z,j}^n) + \\ \frac{p_2c_{\text{ref}}^2\Delta_t^2\Delta_z}{\Delta_y^2(c_{\text{ref}}\Delta_t + p_0\Delta_z)} \left\{ (E_{N_z+1,j-1}^n + E_{N_z+1,j+1}^n - 2E_{N_z+1,j}^n) + (E_{N_z,j-1}^n + E_{N_z,j+1}^n - 2E_{N_z,j}^n) \right\} \quad (\text{A.188})$$

A.15 Continuity equation from time domain wave equation

Before deriving continuity equation from the wave equation, first the terms involved has to be defined. We could generally define a physical quantity q , associated with a flow. q could be mass, energy, electric charge or number of molecules. The associated flow can be defined as mass flow, energy flow or charge flow. In this thesis, q is the energy associated with the wave propagation. Next, we define a term called as flow current, $I(r, t) = \frac{\partial q(r, t)}{\partial t}$ where I is the amount of q flowing at a given time t . Current density $J(r, t) = \frac{I(r, t)}{A}$ is the current normalised to the area A associated with the flow. Current density or flux density $J(r, t)$ is a vector field with dimension $[q/(area \times time)]$. Let $\rho = \frac{q}{V}$, the physical quantity q per unit volume. ρ could be volume density such as mass volume density or energy volume density. Goal in this section is to relate the vector field $J(r, t)$ with the scalar field ρ .

Gauss divergence theorem states that $\int_S J(r, t) \cdot (\hat{n} dS) = \int_V \nabla \cdot J(r, t) dV = q/t = (V\rho)/t$. Local form of continuity equation for a conserved quantity q is given as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot J(r, t) = 0 \quad (\text{A.189})$$

Dimensional analysis : Lets say q is energy (*Joules*), then energy volume density is $\rho = \text{Joules}/m^3$, Current, which energy flow per time $I = \text{Joules}/s = \text{Watt} = \text{Power}$, Current density $J(r, t) = I/A = W/m^2 = \text{Joules}/(m^2s)$. Then for continuity equation, dimensional analysis yields, $\frac{\partial \rho}{\partial t} = \frac{J}{m^3s}$. For $\nabla \cdot J(r, t)$, ∇ operator has a dimension $1/m$ and $J(r, t)$ has a dimension $\text{Joules}/(m^2s)$. Therefore the dimensions match.

A.15.1 The energy method

Multiply both sides of the wave equation

$$\nabla^2 E(r, t) = \frac{1}{c^2} \frac{\partial^2 E(r, t)}{\partial t^2} \quad (\text{A.190})$$

by $\frac{\partial E(r, t)}{\partial t}$ to obtain

$$\frac{\partial E(r, t)}{\partial t} \nabla^2 E(r, t) = \frac{1}{c^2} \frac{\partial E(r, t)}{\partial t} \frac{\partial^2 E(r, t)}{\partial t^2} \quad (\text{A.191})$$

$R.H.S$ can be re-written by chain rule as

$$\frac{1}{2c^2} \frac{\partial}{\partial t} \left[\left(\frac{\partial E(r, t)}{\partial t} \right)^2 \right] \quad (\text{A.192})$$

For the $L.H.S$, the following vector calculus identity need to be used

$$\phi \nabla^2 \psi = \nabla \cdot (\phi \nabla \psi) - \nabla \phi \cdot \nabla \psi \quad (\text{A.193})$$

where ϕ and ψ are scalar fields. Hence equation A.191 can be written as

$$\nabla \cdot \left(\frac{\partial E(r, t)}{\partial t} \nabla E(r, t) \right) - \underbrace{\left(\nabla \frac{\partial E(r, t)}{\partial t} \right) \cdot \nabla E(r, t)}_{\frac{1}{2} \frac{\partial}{\partial t} |\nabla E(r, t)|^2} = \frac{1}{2c^2} \frac{\partial}{\partial t} \left[\left(\frac{\partial E(r, t)}{\partial t} \right)^2 \right] \quad (\text{A.194})$$

Curly underbrace in the above equation involves the use of chain rule for differentiation. Rearranging the equation and comparing it with that of the continuity equation, we get

$$\underbrace{\frac{\partial}{\partial t} \left(\frac{1}{2c^2} \left[\left(\frac{\partial E(r, t)}{\partial t} \right)^2 \right] + \frac{1}{2} |\nabla E(r, t)|^2 \right)}_{\rho(r, t)} + \underbrace{\nabla \cdot \left(-\frac{\partial E(r, t)}{\partial t} \nabla E(r, t) \right)}_{J(r, t)} = 0 \quad (\text{A.195})$$

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