Universiteit Utrecht

Opleiding Natuur- en Sterrenkunde

Simulating Optical Scattering in Disordered Media Using KWANT - Working at the Interface Between Electronic Transport Theory and Optics

Bachelor Thesis

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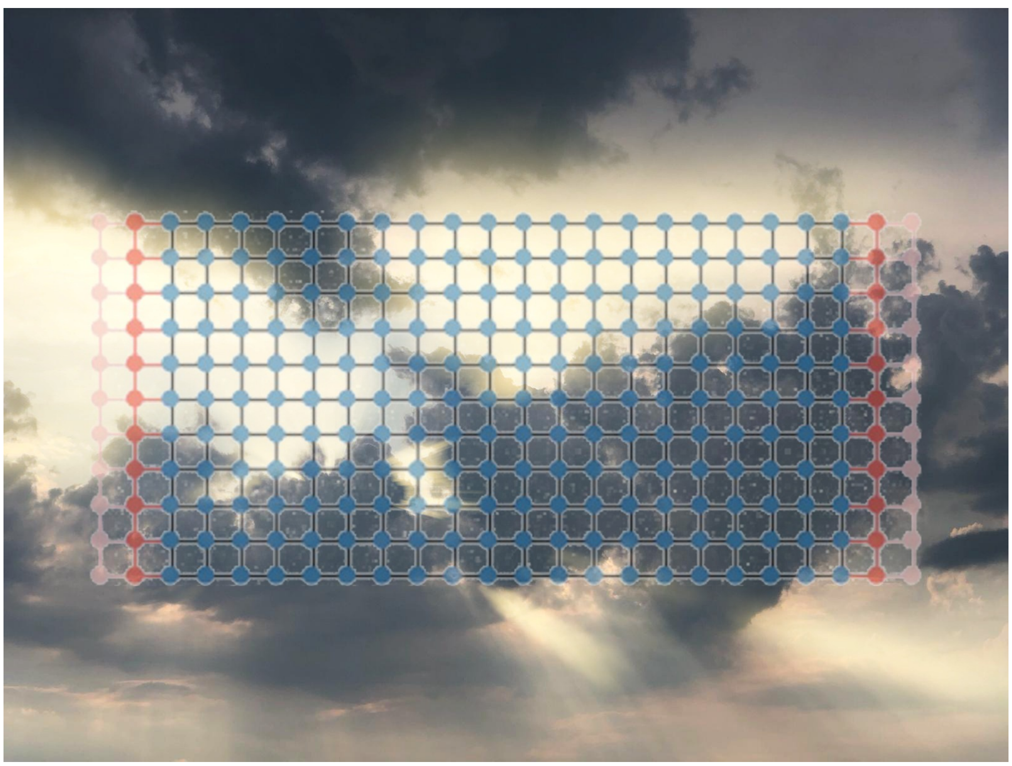

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Abstract

In the past few decades research in light imaging and wave-front shaping techniques have received growing attention. The statistics of the transmission matrix have made it possible to better understand the properties of optical scattering in disordered media and have provided the means to more efficiently propagate light through diffusely scattering media. Experimentally the transmission matrix has successfully been calculated using a spatial light modulator. Numerically, methods for computing the optical transmission matrix exist, however, they are "scattered" in the literature, not very efficient and not regularly updated. KWANT, an open source python package created to compute simulations of electronic transport experiments, has proven to be highly efficient, easy to use, and well-maintained. Motivated by the similarities between the Schrödinger equation and the Helmholtz equation, we compute an optical scattering experiment simulation using KWANT and show that it can in fact be implemented for research in the field of optics.

Front page: The picture on the front page is a photo that was taken on the coast of Greece. The lattice structure was obtained using KWANT and it was edited into the photo.

Contents

Acknowledgement

Firstly, I would like to express my gratitude to my first supervisor, Prof. Dr. Allard Mosk, who, despite the impossibility of meeting in person, provided me with the necessary material and explanations without which I would not have enjoyed as much the process of research and understanding that was required to write this thesis. I feel extremely fortunate to have been given the opportunity to work in a niece topic such as 'wave-front shaping', of which Mosk is a recognized pioneer. Furthermore, I would also like to thank my second supervisor, Dr. Dries van Oosten, for providing me with the necessary remarks and initially guiding me through finding the research most suitable to my interests in a context that, on top of the Covid-19 crisis, was out of the ordinary.

1 Introduction

Light has a fundamental role in the way humans interact with the world. The field of optics marks its origin back to the ancient cultures. In the past few decades experiments have shown the possibility of wave-front shaping and opened new prospects to the fields of imaging and focusing of light and their applications [1–6]. For that reason, the study of the propagation of light through disordered structures has received growing attention. When light travels through media it is scattered and its direction is deviated. If a scattering object is placed between a detector and a light source, depending on how weakly or strongly scattering the object is, the light propagating through the object is distorted. In order to obtain useful information on the distortion one must solve what is referred to as the "scattering problem". The scattering problem is not only pertinent to optics, but it is to all wave phenomena. Similarly to optics, the understanding of the propagation of waves in disordered media is a fundamental aspect of the scattering problem in other branches of physics, such as in solid-state physics and acoustics. There already exists extensive literature on waves propagating in ordered and homogeneous systems ([7, 8]), however, understanding the behavior of waves in more complicated structures is a very difficult task.

For the case of light, the scattering of electromagnetic waves can most exactly be calculated by finding the solutions of Maxwell's equations [8]. Due to the disorder of the medium, however, it is impossible to obtain a solution analytically and attempting to find numerical solutions is extremely inconvenient. A successful statistical tool that has facilitated the manipulation of wave behavior in disordered media is the transmission matrix [2, 9–11]. The transmission matrix is part of the scattering matrix and it includes information about the medium in which the wave propagates. It provides more insight into the medium than using different methods ([1]), and the information that can be extracted from it enhances our ability to manipulate the propagation of waves.

In the case of optical scattering calculating the transmission matrix is a rather elusive problem. In most recent experiments the optical transmission matrix was retrieved using a spatial light modulator [1, 2, 4, 5, 10]. Numerically it is still very challenging to obtain results for a system large enough to resemble real experiments, as the amount of time and memory that are employed to compute those kinds of simulations makes is rather inconvenient. It is then of great interest to look for more convenient numerical methods to retrieve the optical transmission matrix. Reconstructing the transmission matrix is a problem that has been solved in the field of electronic transport. In the case of optics, there exist several numerical methods that have been employed to obtain the optical transmission matrix of a system [12]. They, however, lack in efficiency, and accessibility. The development of a well-maintained, convenient and uncomplicated framework for computing optical scattering experiments would be of great use for research in the field of optics.

Concerning the domain of electronic transport, in 2014 a new open source Python package was created called KWANT [13]. The Python package is well designed to solve the scattering problem in a highly efficient and compact way, and it provides the means for obtaining the transmission matrix of a system. Furthermore, it has proven to compute scattering systems much faster than the other existing methods [13, 14]. It would be of great use to research in optics if it were possible to simulate optical scattering systems with KWANT. Literature has shown that for non-absorptive stationary scattering, when neglecting the effects of polarization is possible, electrons and photons are described by the same wave-equation [1, 4, 15–17]. Because of the similarities among the Helmholtz equation, describing the propagation of light, and the Schrödinger equation, describing the propagation of electrons, it is then possible to work at the interface between electronic transport and optics, and to transfer notions and concepts from one field to another. For that reason we aim to show that KWANT can be used to obtain the transmission matrix of an optical scattering system. We will therefore show that the transmission matrix of a scattering system computed using KWANT provides the statistics that one would expect from an optical scattering system. The ultimate motivation for this research it that of providing convincing enough results such that we can use KWANT for further exploration in the field of optics.

2 Theory

Many phenomena can be described as the propagation of waves. For this reason the problem of wave scattering in disordered media has been addressed from different branches of physics, such as acoustics, electronics and electromagnetism. Obtaining an exact solution to the wave equation is an almost impossible challenge, as even numerically it requires immense computational power. The obstacles that characterize the scattering problem have required theorists and experimental physicists to approach scattering differently. Extensive work in mesoscopic scattering theory has led to the formulation of useful theoretical tools to effectively tackle the scattering problem in the context of electronic transport [1, 15, 18]. The scattering matrix contains information regarding the way a wave has been scattered after it has traveled through a disordered medium and it makes an effective tool in both electronic transport theory and optics. It is necessary to understand where the two subjects meet and the role the scattering and transmission matrix play in them.

2.1 Electronic Transport

From quantum mechanics we know that electrons exist both as particles and waves. Their behavior is characterized by the wave function $\Psi(\mathbf{r}, t)$ which absolute square gives a probability density of the electron. In vacuum an electron behaves as a *plane wave*. Its configuration depends on the quantum states available to the electron, such that

$$\Psi_{\mathbf{k}}(\mathbf{r}, t) = \frac{1}{\sqrt{\nu}} e^{(i\mathbf{k}\cdot\mathbf{r} - iE(\mathbf{k})t/\hbar)}, \tag{1}$$

where $\mathbf{k}$ is the wave vector corresponding to the available state, $E(k) = \hbar^2 k^2/2m$ is the energy corresponding to that state, and ν the volume over which a single electron is spread [18]. In general, the behavior of the electron can most exactly be obtained solving the Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla\Psi + V(r)\Psi, \tag{2}$$

also expressed in terms of the Hamiltonian operator $\hat{H} = -\frac{\hbar^2}{2m}\nabla + V(r)$. In most cases finding a solution to the Schrödinger equation is a very difficult task. There are several instances for which solving it is less difficult. As we are interested in the more general features of electronic transport we will consider a relatively simple case, the *infinite wire*.

Consider a wire of rectangular cross-section. It is infinitely long in the x-direction and it is confined to an arbitrary length by an infinite potential in the y- and z-directions, such that impenetrable walls are created which ensure that electrons cannot escape the wire. As the electrons travel through the structure, when they hit the walls they are reflected. The solution to the Schrödinger equation is given by the superposition of incident and reflected waves. As derived in [18], for such system we obtain the following wave function:

$$\psi_{k_x,n}(x, y, x) = \psi_{k_x}(x)\Theta_n(y, z), \tag{3}$$

such that its horizontal motion is that of a plane wave with $\psi_{k_x}(x) = e^{ik_x x}$, and its tranvserse motion in the y- and z-directions described by $\Theta_n(y, z)$ is *quantized*. The electron can only exist in one of n allowed states. The states that the electrons can take are called *modes* (or *transport channels* in the context of electronic transport), and they characterize the wave function that describes their propagation in the wire. For this reason the wire acts as what is called a *wave guide*, such that to different wave guides correspond different sets of available modes.

From classical wave theory we know that if a wave sent from the left hits a scattering barrier, part of it will be reflected back and part of it will be transmitted. Consider the case of a potential barrier of thickness d and finite size U_0. The electrons propagating in the wire will be reflected or transmitted depending on whether their energy E is smaller or larger than the potential of the barrier. After the electrons are reflected or transmitted

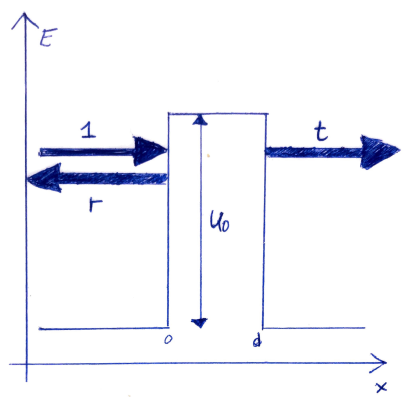


Figure 1: Sketch of wave scattering by a rectangular a potential barrier

they will continue to "freely" propagate in the left or right direction. We then expect that their wave function is given by the superposition of these two cases, such that, for a certain energy, the absolute square of the wave function gives the probability of the electrons being transmitted or reflected. Following the discussion on [18] we define the factors named r and t which represent the reflection and transmission amplitudes of the propagating electron wave (see Fig.1). Their absolute squares give the *reflection coefficient* $R(E) = |r|^2$ and the *transmission coefficient* $T(E) = |t|^2$. They are the fraction of the incident wave that is reflected and transmitted. This constitutes the simplest example of scattering systems of electrons which motion is confined in the transverse direction. In the context of electronic transport the potential barrier is said to act as a *scatterer*. The modes with which the electrons are transmitted in the wire are called *open channels*, the remaining make the *closed channels*. For each channel we can define a *channel-dependent transmission coefficient* $T_n(E)$. For an open channel (a fully transmitted wave) $T = 1$, for a closed channel (a fully reflected wave) $T = 0$.

When we describe electron transport in solids, the main quantity of interest is the conductance. The conductance is a measure of the intensity of the transported current I through a system and the voltage difference V applied to it, such that $G = I/V$. It has been experimentally shown that, when dealing with narrow conductors, as the with of the conductor constraining the electrons is reduced the conductance reduces in discrete steps of height $(2e^2/h)$ (see [15]), as in Fig.2. Solids structures are made of molecules and atoms and they can be

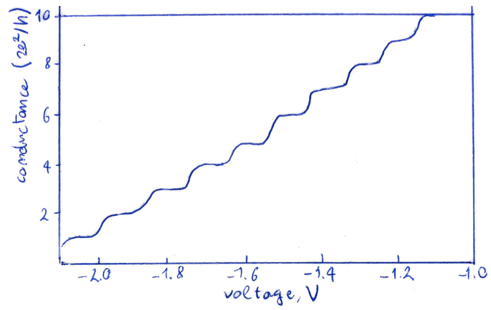


Figure 2: Sketch of the quantization of the conductance G expressed in units of $2e^2/h$.

treated as scattering regions that deviate the trajectory of the electrons that travel through them. The probability that an electron is transmitted is given by the *channel-dependent transmission coefficient* $T_n(E)$. For a fixed energy, the transmitted current must then be proportional to the number of open channels. The relationship among the conductance and the transmission coefficient of a medium is given by the Landauer formula:

$$G(E) = \frac{2e^2}{h} \sum_m T_m(E), \tag{4}$$

such that, at a fixed energy E, each available mode m, if open, contributes one unit of $2e^2/h$ to the conductance. Therefore, in a system in which electron travel “undisturbed”, its conductance will show m steps.[1]. When a wave hits a scattering region, its amplitudes is modified and the initial transverse mode might change into another one. Consider now a system as the one in Fig.3 with the scattering region being solid and the leads two ideal wave guides. The scatterers in this case originate from the defects or impurities within the solid structure, they are randomly distributed and contribute a potential of random size. The wave functions of the electrons take complicated forms in the scattering region and they are impossible to calculate. In the leads however the electrons behave as plane waves that can take a specific set of shapes depending on the available transport channels, so that they can enter and leave the scattering region in that same set of transport channels (see Fig.4). Be N_L and N_R the number of available transport channels to the left and right of the scattering region at a fixed energy E, then there exists a $(N_L + N_R) \times (N_L + N_R)$ matrix that contains information regarding the probability that an electron that hits the scattering region with mode n will be transmitted or reflected with mode m[2]. Such matrix is called the *scattering matrix* and it has the following block structure:

$$\hat{s} = \begin{pmatrix} \hat{r} & \hat{t}' \\ \hat{t} & \hat{r}' \end{pmatrix}. \tag{5}$$

The $N_L \times N_R$ transmission matrix $\hat{t}$ and the $N_L \times N_L$ reflection matrix $\hat{r}$ contain the transmission and reflection amplitudes for electrons propagating from left to right respectively t

[1] further discussion and sources on the matter can be find in [18] and [15].

[2] for further discussion on the scattering matrix and its properties within electronic transport theory see [15, 18, 19].

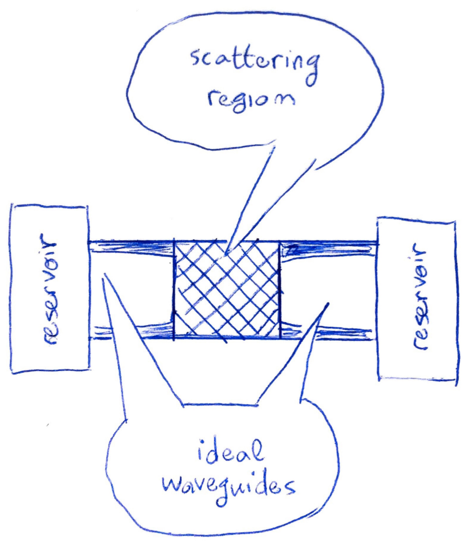


Figure 3: Sketch of the structure of a scattering system to study electronic transport.

and r. The matrices $\hat{t}'$ and $\hat{r}'$ instead account for electrons coming in from the right. The absolute square of each element of the transmission and reflective matrices gives the channel-dependent transmission and reflection coefficients, such that $T_{nm} = |t_{nm}|^2$ and $R_{nm} = |r_{nm}|^2$. It is then clear that once the transmission matrix of a scattering system has been found a lot

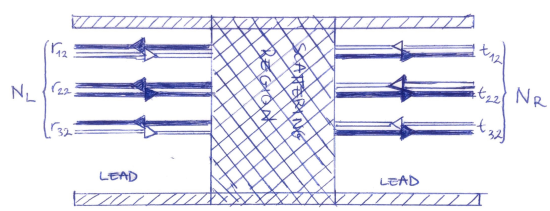


Figure 4: Sketch of the structure of a two-terminal scattering matrix.

of information can be gathered regarding the initial and final state of an electron wave hitting the scattering region, and, in particular, the open channels that will provide the greater transmission can be identified.

2.2 Optical Scattering

In a transparent medium light travels in a straight line: this light is referred to as *ballistic*. However, when it encounters obstacles, two thing happen: part of it is absorbed or its direction is changed, scattered. Depending on the nature of the obstacle and the heterogeneity of the scattering medium, light will scatter differently. When light propagates through many weakly-absorbing obstacles it undergoes what is called *multiple scattering*. Light that travels in a medium and is fully transported undergoing multiple scattering is called *diffusive*, as the energy in the initial beam is converted in a glow of scattered light. In general, for light that travels in a medium of width W, such that the average distance between the occurrence of two scattering events is the mean-free-path l_s, then light propagates ballistically if $L \ll l_s$, and diffusely if $L \gg l_s$. The diffusive behavior of light can be seen looking up in the sky on a cloudy day, such that it is often very difficult to deduce were exactly the sun is located above the clouds. Being able to explain and predict how light is scattered in a medium of arbitrary disorder is done by solving the *scattering problem*.

It is well known that the propagation of light is described exactly by Maxwell's equations [8]. In order to solve the scattering problem, one would have to define a dielectric function $\epsilon(\mathbf{r}, t)$ of the scattering medium, with its positional dependence referring to the location of each scatter [3]. One does not need to point out that, when considering a realistic medium, that is an ambitious and extremely difficult task. Furthermore, numerically it would require an inconveniently long amount of time and memory to bring forth such calculations. On one hand, diffusion theory is well equipped to describe energy transport of classical waves traveling in scattering media [7]. On the other hand however, by using diffusion theory one is only able to obtain ensemble-averaged properties of light propagating in a medium ([7, 9]), and one is only able to predict a smooth interference pattern [4]. Diffusion theory does indeed neglect several features which take place in the mesoscopic and microscopic scattering regimes, such enhanced back-scattering effects and Anderson localization [20]. Experiments have shown that, in the case of diffusion, the only information regarding the scattering of a laser beam is found in interference patterns that are called *speckles*. It has indeed been observed that when monochromatic light undergoes multiple scattering by a medium, the speckles look grainy ([4]), meaning that there exist "open channels" to which light can couple and transport almost "undisturbed" ([21]), or, at least, more light is able to reach the same point. The intensity of a speckle grain at a location is a consequence of the superposition of all the wave amplitudes arriving at that location. Each amplitude corresponds to a mode, such that there will be modes that contribute to speckle grains and other which do not, the former being the open channels, the latter the closed channels. A dark spot means that the resulting amplitude is zero, whereas an intensity maximum is found if all waves superpose at that point. For purely diffusive scattering of light, it can be derived that the speckle intensity probability distribution takes that of a negative exponential, such that the ration between the square of the standard deviation and the mean of the intensity gives a *normalized variance* $D = \sigma_I^2/\bar{I}$=1 [6, 22].

The preferred approach to the scattering problem is to find a tool that relates the field of the light coming in to that of the light coming out of the scattering region. From the discussion in the previous chapter we know well that such a tool exists and it is the scattering matrix. In particular, in optics one is interested in the transmission matrix $\hat{t}$, which is found in the scattering matrix as indicated in Eq.5, and relates the set of allowed input modes to that of allowed output modes, such that

$$E^{out} = \hat{t}E^{in}. \tag{6}$$

Specifically each incident field in channel n and outgoing field in channel m make a linear combination of all contributions N to the output channel, such that

$$E_m^{out} = \sum_n^N t_{mn} E_n^{in}. \tag{7}$$

The transmission coefficients are only valid if the system is static. Their distribution must obey the same statistics of the speckle intensity distribution as they are related to the resulting intensity of the scattered light [3]. For scattering in a homogeneous, ordered sample, we expect that the optical transmission matrix takes the form of an identity matrix, i.e. for each channel light travels through the medium undisturbed. For scattering in the diffusive regime we expect the distribution of the values of the components of the transmission matrix to decay exponentially, as it does for speckle intensities. Having established the role of the transmission matrix in electronic transport theory and optics, we can demonstrate where the two fields come into contact.

2.3 Analogy between Electronic transport theory and Optical Scattering

There exist a good amount of literature that outlines the similarities among electronic transport theory and optical scattering, both theoretically ([1, 4, 15, 16]) as well as experimentally [17]. The starting point is that the structure of the Schrödinger equation, describing the propagation of electrons,

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{i\hbar^2}{2m}\nabla\Psi + V\Psi, \tag{8}$$

and the Maxwell equation, describing the propagation of photons,

$$\frac{\partial^2\mathbf{E}(\mathbf{r},t)}{\partial t^2} = \frac{1}{\mu\epsilon}\nabla^2\mathbf{E}(\mathbf{r},t), \tag{9}$$

are very similar. The greatest difference stands in the fact that the wave function $\Psi(\mathbf{r},t)$ is a statistical quantity and it provides a probability density, whereas the field $\mathbf{E}(\mathbf{r},t)$ is a measurable macroscopic vector quantity that gives an intensity.

For a system of stationary states and a well defined energy E_0, using the definition of momentum operator $\mathbf{p} = -i\hbar\nabla$, the Schrödinger equation takes the following form:

$$\left(\nabla^2 - \frac{2m}{\hbar^2}[V(\mathbf{r}) - E_0]\right)\psi_E(\mathbf{r}) = 0. \tag{10}$$

On the other hand, in a source-free, linear and frequency-independent dielectric medium with dielectric function $\epsilon(\mathbf{r})$, we can obtain the Helmholtz equation in scalar form,

$$\left(\nabla^2 - \frac{\omega^2}{c^2}[1 - \epsilon(\mathbf{r})] + \frac{\omega^2}{c^2}\right)\psi_\omega(\mathbf{r}) = 0, \tag{11}$$

as derived in [1]. It is known that electromagnetic waves in a dielectric medium behave similarly to electrons in a potential. With this clarification we see that to each quantity in Eq.11 cna be found a corresponding one in Eq.10, which also implies that both equations have the same solutions. Furthermore, In the case of the potential $V(\mathbf{r})$ that vanishes, and of light propagating in vacuum, such that $\epsilon(\mathbf{r}) = 1$, we see that both equations have the same solutions. In the case of a well-defined energy, for example, their solution is of the same exponential form as in Eq.1. To this extent the analogy holds for very limited cases as many microscopical properties of light scattering can only be obtained through Maxwell's equations and electrons and light scatter differently. In particular the dispersion relation is quadratic in the electronic case, whereas it is linear in the optical case. That implies that their scattering behavior as a function of time cannot be treated analogously. Nevertheless, for the case of stationary scattering, polarization does not play an important role [1]. As we are interested in obtaining statistics of the scattering amplitudes of electrons traveling through a stationary medium, the analogy among electronic and optical scattering should hold. By using a method intended for electronic transport, we can expect to obtain a transmission matrix that displays, to some extent, the statistics relative to the optical case.

3 Numerical Methods

KWANT is designed to simulate calculations on tight-biding models[3]. Using KWANT in Python, it is possible to construct scattering systems consisting of a finite scattering region which shape and dimension can be set arbitrarily, and attach to it semi-infinite leads. Those leads act exactly as the ideal wave guides from which the radiation comes in and hits the scattering region, similarly to the example in Fig.3. In KWANT the tight-bidning model is applied to a lattice structure such that the Hamiltonian is discretized and is represented as an "annotated infinite graph" with each node corresponding to a lattice point [13]. After a tight-binding system has been created, the calculation of, for example, the transport properties of the lattice is passed to a *solver*. The transmission matrix of the system is directly calculated by the solver, and can easily extracted from the program.

3.1 Framework of the Simulation

In order to asses the possibility of KWANT being able to provide useful results in optical scattering simulations we aimed to reproduce those elements whose statistics we could compare to the theory. We computed the transmission matrix of a 2-dimensional crystal lattice. The theoretical framework of this system is very similar to that of the infinite wire discussed above. The Hamiltonian of a two-dimensional lattice takes the following form:

$$H = \frac{-\hbar^2}{2ma^2}(\partial_x^2 + \partial_y^2) + V(y). \tag{12}$$

The light is confined to the lattice structure by the hard-wall potential $V(y)$, such that the lattice acts as a wave guide. Each lattice point is separated by an arbitrary lattice constant a. In this way the Hamiltonian is discretized, and it can be solved as it is custom for a the tight-binding model for which each lattice point contributes an energy to the Hamiltonian, and the interactions with the neighbouring sites are accounted for by appropriate corrections (see more in [13]). As it is custom workflow with KWANT, we firstly created a tight-binding system and set its on-site and hopping energies. We set that each lattice point has an onsite potential of $4t$ and a closest neighbour correction of $-t$, with $t = \frac{-\hbar^2}{2ma^2}$ being the energy term in the Hamiltonian of Eq.12. For simplicity we set $t = a = 1$. In order to test the accuracy of the code we initially built a dummy rectangular lattice of length $L = 20a$ and width $W = 6a$, such that in Fig.5. The red parts indicating the semi-infinite leads attached to each side acted as the ideal wave guides in which the light propagates to come in, and come out of the lattice. The incoming light is then confined in the transverse direction and for each energy the photons can only take a specific number of modes, which maximum is that equal to the width of the lattice. At this point we had a homogeneous lattice structure with which we could attempt to simulate the behavior of light and obtain a transmission matrix for the system. From theory we know that light traveling in a homogeneous structure propagates ballistically.

In order to test how KWANT simulated the diffusive light we were required to add scatterers to the system. That was done by making the system in-homogeneous, or impure,

[3]The tight-binding model has proven a very successful method in describing the interactions among particles in a solid and crystal structures [7, 15, 23].

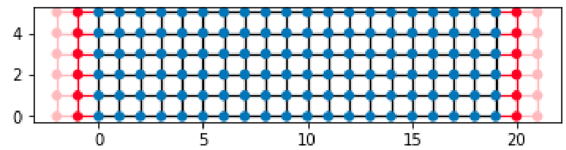
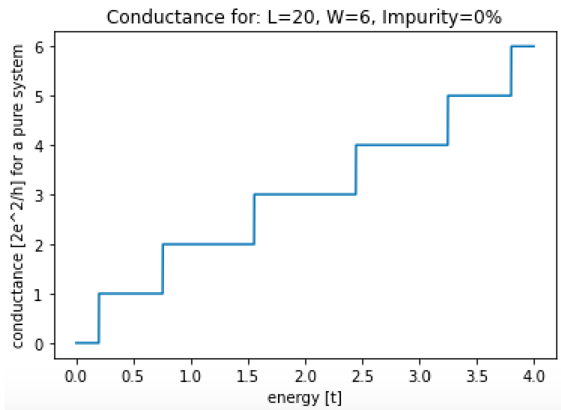


Figure 5: Rectangular lattice six lattice-points wide and twenty long, indicated by the color blue, and the semi-infinite leads attached to both sides indicated by color red.

so by adding a certain degree of disorder in the lattice. From the theory, we knew that disorder in a medium acts as a finite potential $V \neq 0$ randomly distributed among the lattice points. We decided to assign to each point a 1% probability of it being added an attractive potential $V = -0.5t$ to its on-site potential, such that the lattice had an impurity amounting to 1% of the medium. Furthermore, it was necessary to increase the length of the lattice, such that we could simulate light (or electrons) traveling a greater distance before being "detected". In order to be able to asses for which size the system behaved fully diffusely as well as to see whether any interesting trends occurred, we tested the scattering system for various lattice lengths, which ranged between structures long 16 to 12000 lattice points. In particular we hoped to obtain a transmission matrix whose the elements would show a distribution of the form of an exponential decay, which is ultimately the result that is found when light behaves diffusely in a medium. In order to obtain more accurate results, for each lattice length we gathered 1000 transmission matrices and plotted the distribution for the values of the elements of the matrices. In order to differentiate the ballistic, semi-ballistic, and diffusive regimes we treated diagonal and off-diagonal elements separately.



(a)

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[[1. 0. 0. 0. 0. 0.]
 [0. 1. 0. 0. 0. 0.]
 [0. 0. 1. 0. 0. 0.]
 [0. 0. 0. 1. 0. 0.]
 [0. 0. 0. 0. 1. 0.]
 [0. 0. 0. 0. 0. 1.]]
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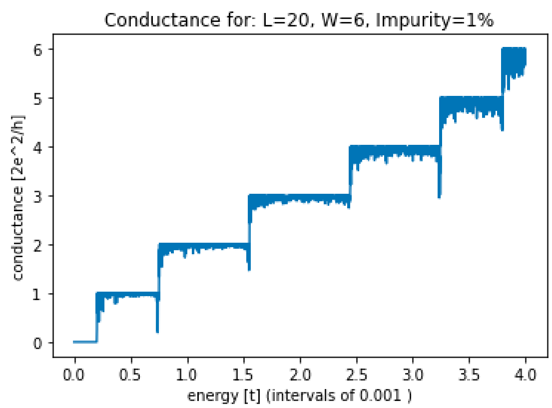
(b)



(c)

```
[[0.964  0.024  0.0796 0.0411 0.049  0.133 ]
 [0.0483 0.97   0.0761 0.0785 0.0672 0.104 ]
 [0.106  0.0631 0.964  0.0631 0.0806 0.119 ]
 [0.0411 0.0843 0.0809 0.95   0.0764 0.143 ]
 [0.076  0.0605 0.0872 0.0634 0.973  0.0972]
 [0.125  0.103  0.106  0.147  0.0889 0.895 ]]
```

(d)

Figure 6: (a) Conductance graph and (b) transmission matrix for a homogeneous scattering lattice; (c) Conductance and (d) transmission matrix for a scattering lattice with impurity of 1%. Of the transmission matrix elements it was taken the absolute up to three significant figures and each, and it was rounded to zero any values less than 10^{-10}.

4 Results and Discussion

4.1 The Ballistic and Diffusive Regimes

The first objective of this research was to extract the transmission matrix from the solver. For a pure system we expected the transmission matrix to be the identity matrix. For a homogeneous system of six lattice points wide, we obtained a conductance graph that showed six steps, and we were able to extract a 6×6 transmission matrix. The results are shown in Fig.6. As the calculation of the transmission matrix with KWANT gave its elements in complex form, we took the absolute of each element to obtain real transmission amplitudes. Furthermore, for the sake of clarity we approximated each element of the order smaller than 10^{-10} to zero. As we can see from Fig.6(b) the transmission matrix we extracted, when approximated and taken the absolute value of its elements, was indeed equal to the identity matrix we were expecting. That is appropriate as it means that for a homogeneous system, for each of the six modes n in the left lead and m in the right lead, there exists a respective transmission coefficient t_{mn}, such that Eq.7 would essentially simplify to

$$E_m^{out} = \delta_{mn} E_n^{in}, \tag{13}$$

which represents the ballistic behavior of light. When adding the scatterers to the same system by setting the impurity of the medium to 1%, we obtained the transmission matrix shown in Fig.6(d). Because of scattering events taking place, the amplitude of the light outgoing the scattering region in the same mode it came in is reduced, meaning that the diagonal elements of the impure system should be smaller. Furthermore, when light is scattered, the original mode with which the wave entered the scattering region will change, such that the amplitude of light coming out of the scattering region in a different mode will be greater and less waves will "freely" propagate through the lattice, meaning that the off-diagonal transmission amplitudes of the impure system should be larger than those for a homogeneous system. If we compare the transmission matrices for the ideal and impure cases in Fig.6, we indeed see that for the impure system the off-diagonal elements are significantly larger, and the diagonal elements are smaller, even though still very large, than those for the homogeneous case.

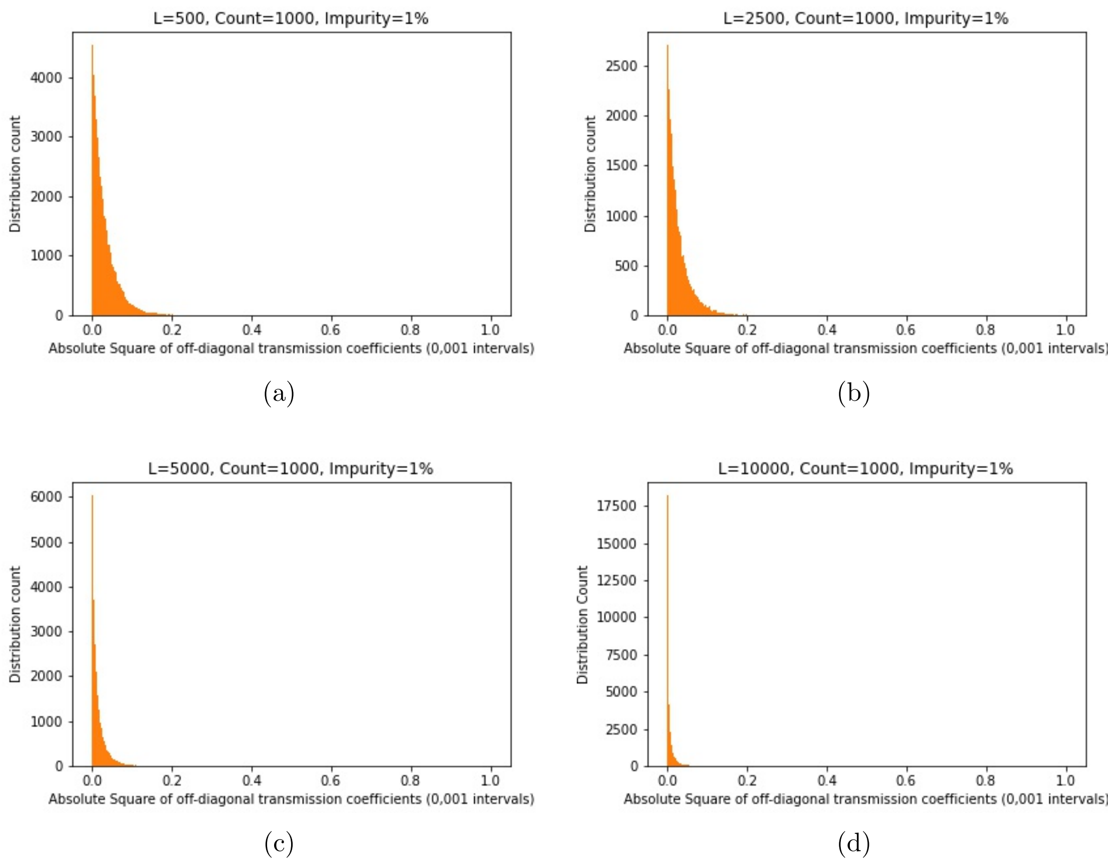


Figure 7: Distribution count of square absolute of the off-diagonal elements of 1000 transmission matrices for (a) L=500, (b) L=2500, (c) L=5000 and (d)L=10000.

In the impure system, light does not propagate freely anymore, however, as the diagonal transmission amplitudes are much greater than the off-diagonal amplitudes, the ballistic light is still prevalent.

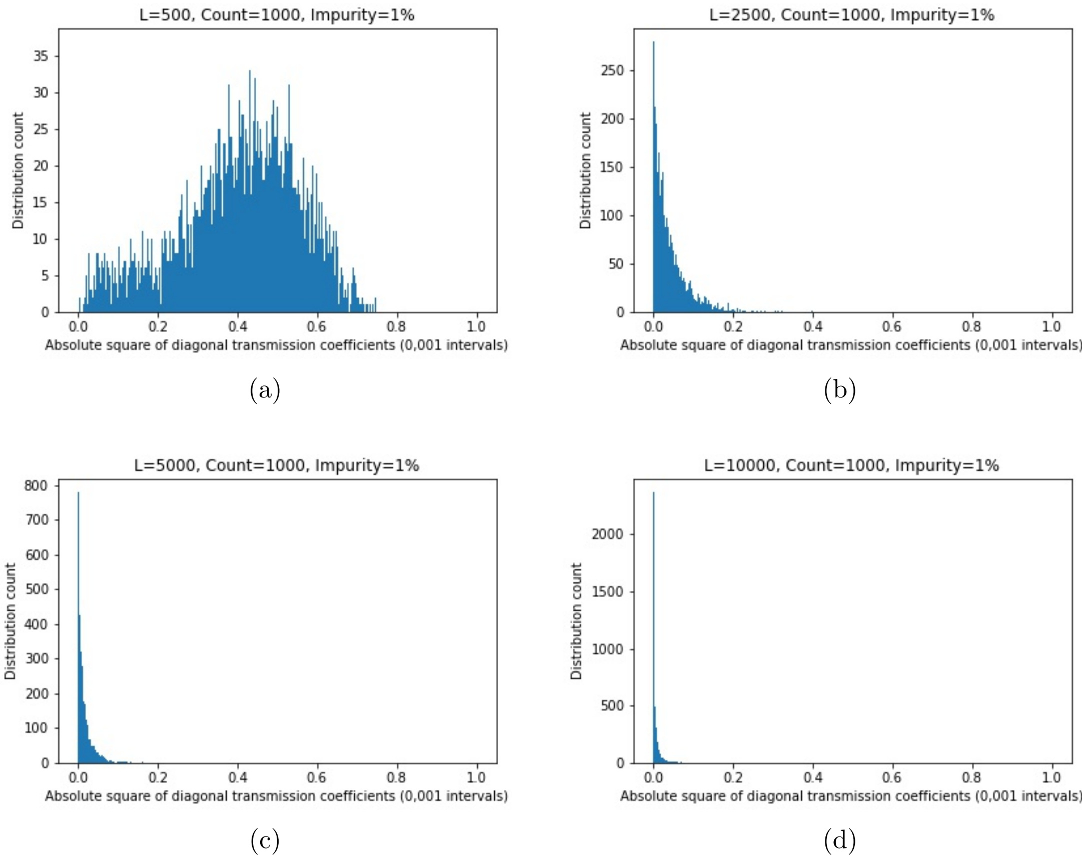
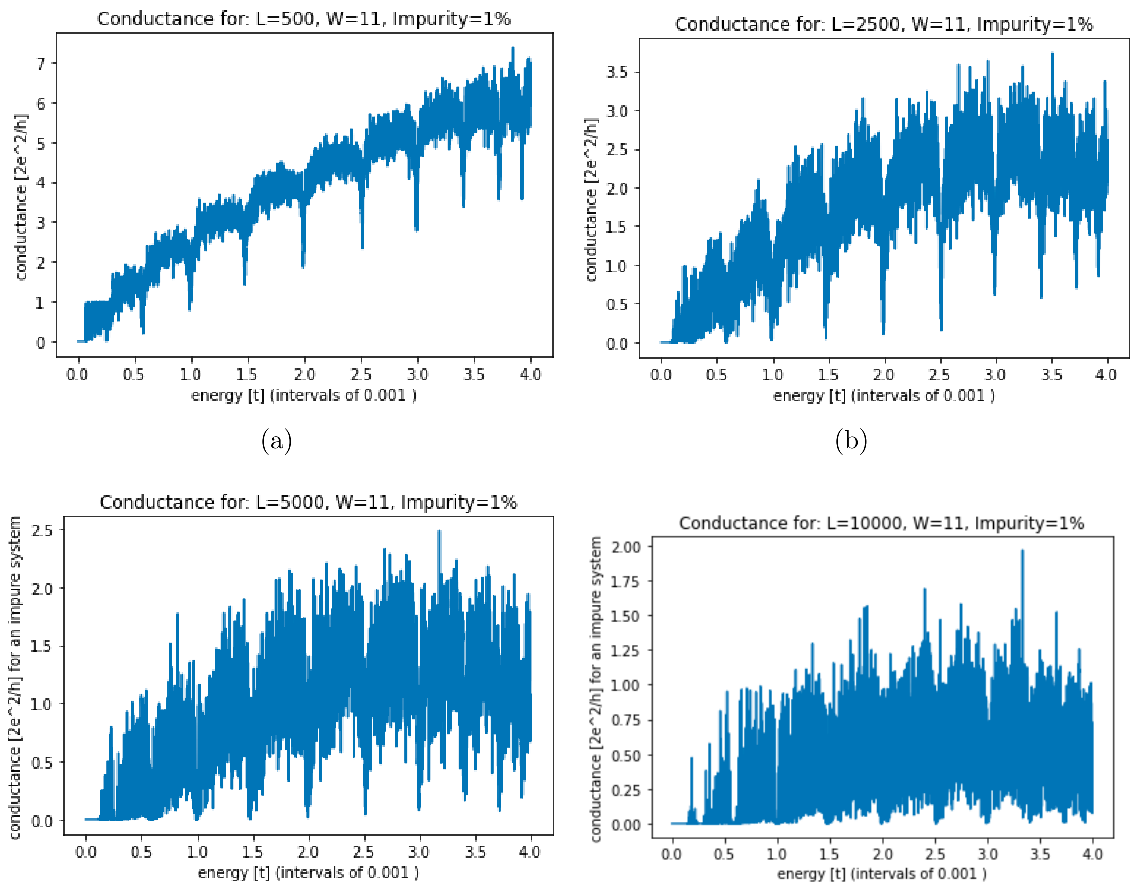


Figure 8: Distribution count of square absolute of the diagonal elements of 1000 transmission matrices for (a) L=500, (b) L=2500, (c) L=5000 and (d)L=10000.

In order to reduce the ballistic light we were required to increase either the impurity, or the length of the system. As it was convenient to compare some of our results with [24], we decided to maintain the same degree of impurity (1%), build a system 11 lattice point wide, and calculate transmission matrices for lengthier systems, with the ultimate goal of obtaining results that could well represent the diffusive regime of optical scattering. For over twenty-five lattice lengths ranging from 16 to 12000 we plotted the distribution of the transmission coefficients of 1000 transmission matrices calculated for each length, and treated the diagonal and off-diagonal cases separately. Some of the plots we obtained are shown in Fig.7 for off-diagonal and in Fig.8 for diagonal elements, as well as the conductance graphs for those same systems in Fig.9. To identify the size of the lattice in which light would scatter diffusely, we needed to obtain a distribution of both diagonal and off-diagonal transmission coefficients that decayed exponentially. In Fig.7 we see that for the lattice lengths 500 and 2500 the distribution of the off-diagonal elements resembles that of an exponential decay. Most transmission coefficients take values close 0, with maximum values around 0.2. That



(a) (b) (c) (d)

Figure 9: Conductance graphs for scattering through a rectangular lattice of width $W = 11$ and length (a) L=500, (b) L=2500, (c) L=5000 and (d)L=10000.

means that for those systems most light that is scattered propagates diffusely. The two cases are however very different in their distribution of the diagonal transmission coefficients. For $L = 500$ we see that they are greatly spread, and they take values ranging from 0 to more than 0.7. That means that many photons propagate through the medium ballistically or semi-ballistically. For $L = 2500$ the diagonal transmission coefficients show a distribution close to that of an exponential decay. For $L = 5000$ and $L = 10000$ we see that the number of transmission coefficients that take value 0 has increased drastically, meaning that very little light has propagated through the medium. By looking at Fig.9 we are able to see the number of open channels available to the photons for each sample. If for $L = 2500$ there are about 3 channels open, for $L = 5000$ there are 2 and for $L = 10000$ only 1. One open channel means that only one photon, or one wave, can travel through the medium. When the conductance reduces to this extent the amount of radiation that propagates through the medium is too little for the statistics of the transmission matrix to provide valuable results.

In order to evaluate whether we could find a system that, to the best accuracy, simulated the diffusive regime of optical scattering, we computed the normalized variance of the distribution of the transmission coefficients for each length. We expected that we could find a

Normalized variance obtained for:							
Lattice L	1000	1500	2000	2500	3000	3500	4000
Diagonal	0.369909	0.642945	0.939526	1.11198	1.30945	1.33973	1.46089
Off-diag	0.961478	1.00905	1.05637	1.11669	1.25858	1.29322	1.40918

Table 1: Table for normalized variance values for different lattice lengths.

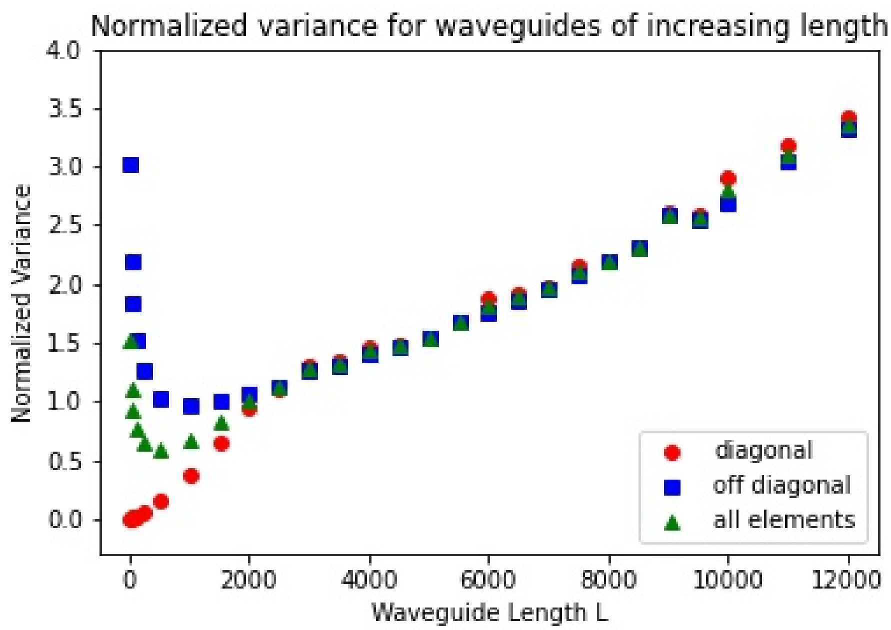


Figure 10: Normalized variance for lattice lengths ranging from $L = 16$ to $L = 12000$ for off-diagonal, diagonal, and all elements of the transmission matrix as indicated by the legend.

system that showed a normalized variance close to 1 for both diagonal and off-diagonal coefficients, and a conductance with a maximum greater than 2. The plot we obtained is shown in Fig.10 and some interesting values are shown in Tab.1. As we can see in Tab.1 the diagonal and off-diagonal elements converge up to two significant figures for $L = 2500$. Beyond that size, the normalized variances of the diagonal and off-diagonal distributions stay close and grows slowly. For $L > 5000$, even though the diagonal and off-diagonal coefficients distribute similarly and their normalized variance is statistically close enough to 1, the conductance available to such systems is too little and the medium does not have enough open channels for a scattering experiment to be able to provide useful results. On the other hand, as we can see from Fig.10, for $L < 2500$, the shape of the distribution of the diagonal and off-diagonal elements diverges fairly quickly. As shown in 1, at $L = 2000$ the normalized variances for the diagonal and off-diagonal cases have already slightly diverged, however, they are still very close to 1. For systems with a length below 2000, the diagonal transmission coefficients spread and take larger values than the off-diagonal elements, showing a distribution similar to that in Fig.10(a). For those systems the diagonal coefficients begin to show the ballistic scattering of light, and their statistics cannot be used to test for diffusive light.

4.2 The Optimal Diffusive Length

In Fig.10 we can clearly see how the scattering regime of light is related to the length of the medium. Until the normalized variance of the diagonal and off-diagonal distributions at a length do not meet, light propagates ballistically in the medium. That means that the lattice is not long enough for two scattering events to take place before light has come out of the scattering region, meaning that its length is smaller than the mean-free-path l_s of the propagating light. For very short lengths light does indeed propagate almost purely ballistically, such that $L \ll l_s$. As the system grows longer, the value of the normalized variance for the diagonal and off-diagonal distributions approaches 1. For a rectangular lattice of width $W = 11$ and impurity 1%, that is the case at its best at about $L = 2500$ lattice points. In other words, in KWANT, a rectangular lattice 11 points wide and 2500 long, with an impurity of 1%, makes the system that simulates diffusive light most appropriately. We call this length the *optimal diffusive length*. It can therefore be argued that: on one hand, for a system with greater impurity, we expect that the value of the optimal diffusive length would shift to the left, meaning that the diffusive regime best occurs at a shorter length. On the other hand, for a system of greater width, as more open channels exist, we expect that the value of the optimal diffusive length would shift to the right. That implies that, in principle, using KWANT, any system can be built such that the *optimal diffusive parameters* can be found to test the diffusive scattering of light. In this view, within the boundaries in which the analogy between electronic transport theory and optics is valid, KWANT can then be used to calculate the transmission matrix of an optical scattering system.

5 Conclusive Remarks

In conclusion, wave-front shaping is a fundamental aspect of focusing light in disordered media. Light imaging has applications in a wide variety of scientific fields. It is of great importance to provide better tools make it easier to bring forth research in optics. The transmission matrix has proven a very useful tool for the understanding of the behavior of waves in a scattering system. A convenient and well-maintained numerical method that can be used to calculate the optical transmission matrix had not yet been found. Enlightened by the similarities between the scattering properties of photons and electrons, we employed KWANT, a python package created to provide calculations for electronic transport systems, to obtain the transmission matrix of a scattering structure, and evaluate if it could accurately reproduce the statistics of an optical transmission matrix.

We were indeed able to show that the transmission matrix calculated with KWANT reproduced the statistics expected for an optical scattering experiment. We built a rectangular lattice of width $W = 11$ and impurity of 1% and tested it for different lengths. We obtained the following results. Firstly, for the case of a pure system, we obtained a transmission matrix that had the form of the identity matrix, and reproduced the ballistic propagation of light. Secondly, by adding scatterers to our system and testing it for increasing lengths, we were able to obtain data that showed the scattering regime of light to go from ballistic to diffusive, and we were able to identify a size range within which light scattered diffusely to a satisfactory extent. We found that to be the case for lengths included between 2000 and 5000 lattice points. Thirdly, we identified an optimal length such that our system simulated the diffusive regime of light scattering to a very good extent. We called that the *optimal diffusive length*. For our system the optimal diffusive length was found at $L = 2500$. Finally, we have argued that, in principle, the optimal diffusive parameters such as size, disorder, and shape of a system, of any dimensionality, built using KWANT, can be found. That implies that, within the boundaries in which the analogy between electron transport theory and optics stands, KWANT can always be used to compute the optical transmission matrix of a scattering system. It is with this conclusion that we hope to motivate the usage of KWANT for more and less advanced research in the field of optics.

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