Monte Carlo Simulation of Light Scattering on a Sound Wave

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Abstract

The theoretical description of light propagation in turbid media has attracted considerable interest. One of the major reasons for that is its high potential in the field of medical imaging. The key problem of the theory of the light propagation in turbid media is the multiple scattering. On its way through the medium light suffers multiple scattering processes. The statistical nature of these processes finally results in the partial or total loss of information of the path of the light through the medium. Various techniques were suggested to bypass this problem such as ballistic photons, coherence techniques or amplitude waves. Ultrasound-assisted optical imaging refers to the cross-modulation of coherent light in a diffusing medium by an ultrasound beam. This effect permits scattered light that has traversed a specific localized region to be distinguished from all other diffused light independently of the amount of scattering both have endured. It therefore provides the possibility of measuring the optical properties of deeply buried objects that cannot be directly discerned.

An advanced novel method to calculate the spatial distribution of the light after interaction with the ultrasound field, in the presence of the optical scatterers, is presented here. The propagation of the light beam through the thin ultrasound slab where thickness is less than one optical transport mean free path resembles realistic situation where light is interacting with the tightly focused ultrasound in biological tissue. Only one mechanism of the ultrasonic modulation of the scattered light was considered. This mechanism is based on ultrasonic modulation of the index of refraction, which causes a modulation of the optical path lengths between consecutive
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scattering events.

The scope of this work includes a derivation of the modified Monte Carlo method of the sound-modulated light propagation in a turbid medium. The classical Monte Carlo model([8], [9]), based on random walk of the photons, was modified and the phase information was included.

The concept under investigation in this project is to add frequency marks to the light by interaction with the sound wave. One option to detect the frequency marked photons is interference. The final goal of this project is to develop a theoretical model (Monte Carlo model) on the propagation of frequency marked photons in a turbid media and to analyze its detectability.

The present work was divided in several parts, the chapters 1–4 are theoretical and the large chapter 6 contains results form the numerical experiments.

In the beginning of the theoretical part of the present thesis we describe some optical properties of a turbid medium (section 1). In the section 2 "A bit of probability theory" some concepts from the probability theory, used in classical Monte Carlo method, are discussed. The classical Monte Carlo model of the light scattering in a random medium is presented in the section 3. Then the basic algorithm of Monte Carlo model light propagation in a random media is considered. The short review of the application of the classical Monte Carlo method is also given in the section 3. After the introductory part we present the novel modified Monte Carlo method to calculate the spatial distribution of the diffused light after interaction with the sound field. The theory about "Light and Sound Interaction" is presented in section 4.

We carry out the numerical experiments (section 5)in several phases, at first we consider the simplest model with the scattering allowed only in a sound beam, as the next step we plug in the optical scatterers in the region before the sound field, and the last step is to consider the effect of scattering in the region after the sound beam.
Motivation

Imaging through a turbid media has in recent years become a field of immense research, mainly due to its great potential for medicine. Most of the difficulties one faces when rendering the turbid medium imaging are related to the random multiple scattering of light.

It is assumed, that light transmitted through a turbid medium contains three components: ballistic, quasi-ballistic light and diffused light. Ballistic light experiences no scattering and thus travels straight through the medium. It carries direct imaging information as X-rays do. Quasi-ballistic light is slightly scattered light and includes most imaging information. Multiply scattered light carries little direct imaging information and overshadows ballistic and quasi-ballistic components. As the thickness of the medium increases the ballistic component of the transmitted light decays exponentially, and the direct imaging information can totally vanish. Quasi-ballistic and diffused light exhibits a random walk like behavior during its propagation in turbid media, that commonly makes standard back projection algorithms impossible to apply.

It is known that photons which have been scattered a small number of times carry more spatial information than diffuse photons. Methods which can isolate minimally scattered photons from the diffusely scattered background, such as collimated detection, coherent technique and time-gating were reviewed in detail by [15]. However, the fraction of minimally scattered photons transmitted across large (greater than several centimeters) thickness of the of turbid medium is immeasurable small, making this
Motivation

approach unsuitable for medical imaging. The length scale over which a collimated beam becomes diffuse is known as the transport scattering length, which is about $1 - 2\text{mm}$ in most biological tissues at NIR wavelength. The focus in majority of the experimental works was on measuring and identifying minimally scattered photons, which cannot be applied to a turbid medium more than a few millimeters thick [15], [16].

Since the intensity of diffuse light decreases significantly slower with increasing opacity, there has been intense interest in using diffuse light for imaging of strongly scattering structures. The challenge of achieving high-resolution imaging with diffuse light has stimulated a variety of approaches. The main distinction between different optical models, where diffuse light is used, is how they collect data from which the image information is constructed. The form in which data should be collected is a major consideration for the researches.

Ballistic Imaging. Early Photon Imaging

If diffused light is rejected and ballistic or quasi-ballistic light is collected, buried objects can be detected and this method is called ballistic imaging. Diffraction-limited resolution in imaging through turbid media requires the detection of ballistic light and the rejection of most of the scattered light. Efficient methods for accomplishing this goal, including time-resolved techniques and heterodyne detection, have recently been explored [18].

Temporal imaging techniques (time-resolved techniques) rely on the fact that the ballistic light will be the first light to arrive at the detection apparatus while the multiply scattered component will be significantly delayed, providing the necessary rejection. Various time-of-flight detection schemes have been used including streak camera, coherent temporal gating, nonlinear gating, etc [15]. Only the initial portion of transmitted light is allowed to pass to a light detector, and the late-arriving light is gated off by a fast optical gate [19].
In contrast to time-resolved methods, spatially resolved techniques rely on directional selectivity to suppress the diffuse component of the transmitted light [18]. Spatially resolved techniques include optical heterodyning and confocal imaging. While effective, these spatial techniques may have difficulty rejecting light that has been multiply scattered back into the ballistic direction.

The time domain technique requires expensive short–pulse laser and fast light detectors [4]. It has been shown that ballistic imaging is feasible only for medium thickness less then 1, 4mm [4]. Therefore, this approach is suitable for thin medium but suffers loss of signal and resolution for thick medium as a result of a strong scattering by the tissue.

**Optical Coherent Tomography**

Optical Coherent Tomography uses ballistic and near–ballistic photons [20], [21], [17]. Laterally adjacent depth-scans are used to obtain a two–dimensional map of reflection sites in a sample [17]. This system consists of an interferometer which is fed by a broadband light source. The light beam is splitted passing through the interferometer and is directed to two different paths, the reference and the sample parts. The reflected beam from reference mirror and the one from scattering sample (turbid medium) then go back to the interferometer and generate a cross-correlation signal which is directed towards a detector. The detection of interferometric signal is possible only when the sample and reference signals are almost matched in time of light (group delay). In this technique the interference of the reference beam and the beam passed through the sample is used.

As shown above, various techniques were investigated to overcome the problem of the multiple scattering of light in a random medium. All this approaches are used for thin turbid media because the ballistic or quasi-ballistic photons can be detected. For practical purposes the turbid medium of thickness 5-10 cm is used, the detector must collect transmitted light that has experienced at least 1100 scattering events inside the media [4]. Therefore ballistic and even quasi-ballistic light provides very low
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contribution to the transmitted signal.

Diffuse Optical Imaging

At depths from approximately 3 – 5\text{mm} up to 8 – 9 \text{cm} multiple scattering dominates in light propagation in turbid media. Under these conditions, optical phase relationships become randomized and coherent properties are not detectable. In this "Diffusion regime", light transport can be modeled as a diffusive process where photons behave as stochastic particles. Under these conditions quantitative tissue measurements can be obtained by separating light absorption from scattering using time- or frequency – domain techniques. The underlying physical principles of these methods are based on the fact that light absorption, which is a consequence of light and molecules interactions, take place on a slower time scale than light scattering. Thus, these processes can be resolved by a time– or frequency – domain measurement [22], [24].

The frequency-domain imaging has been designed to evaluate the dynamic response of scattered light intensity to modulation of the incident laser beam intensity, in a wide frequency range and is also called photon density wave imaging [23],[24]. This method measures the modulation depth of scattered light intensity and corresponding phase shift relative to the incident light modulation phase. However this technique suffers from the simultaneous transmission and reception of signals and requires special attempts to avoid unwanted cross-correlations between the transmitted and detected signal. This technique uses amplitude-modulated laser light (at approximated 100MHz) to illuminate the tissue and detects the diffused light.

In addition to techniques based on the clear imaging of a turbid media, there exist other methods often referred to as hybrid techniques. A promising concept in hybrid techniques is the tagging of light by ultrasound [1], [2]. The light modulated by a sound wave inside the random media can
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Figure 1: A typical configuration of an acousto–optical experiment in a turbid medium

be discriminated from diffused transmitted light by various methods.

Ultrasound-Modulated Optical Imaging

A typical configuration of an acousto–optical experiment in a turbid medium is shown in figure 1. An ultrasound wave that may or may not be focused propagates in a turbid medium. The ultrasonic wave modulates light passing through the ultrasonic field. The scattering of ultrasound in the medical frequency range is low. The position of ultrasound rays in the turbid medium is therefore well determined. Consequently, the origin of light marked by an ultrasound is also known.

Light crossing the volume with the sound field is phase modulated because the ultrasound modulates the optical path through both a change of the refractive index of the medium and a periodic motion of the scatterers. The later corresponds to a frequency shifting of the photons involved and is often referred to as photon tagging [25].

The concept of acousto–optical (AO) imaging relies upon an interference
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measurement between these tagged photons and coherent photons that have not crossed the sound field. It is free of the hazards of ionizing radiation associated with mammography and separates the resolution and signal problem of light-only imaging because the resolution is determined by the size of the ultrasound focus and the signal depends on any light passing through the ultrasound focal zone. When the ultrasound scan points out a volume presenting an optical contrast (local absorbance and/or scattering properties) like tumors, the quantity of tagged photons is modified. Localization and resolution (1mm) of objects are made possible because of the good directionality of the ultrasound within biological tissues [26].

Light propagated through a turbid medium can be tagged by the continuous-wave ultrasound [4] or by pulsed ultrasound [25]. In [25] the combination of pulsed ultrasound and laser light is used, and the ultrasound-modulated optical signal without buried objects is detected. The model proposed by L.Wang in [4] images buried objects in tissue-simulated turbid medium using continuous-wave ultrasound–modulated optical tomography. The major advantage of continuous-wave ultrasonic modulation over pulsed ultrasonic modulation is the significant increase in signal-to-noise ratio which allowed one to image buried objects in turbid media.

Several theoretical models were developed to describe the interaction of ultrasound with light in biological materials. Mahan et al. [3] presented a theory to predict the detection efficiency of diffused light whose frequency is modulated by an acoustic wave. Wang [4] identified the following three possible mechanisms for ultrasound modulation of light in a scattering medium: The first mechanism is based on ultrasonic-induced variations of the optical properties of the medium such as the variation of the absorption and the scattering coefficient, figure 2. The second mechanism is based on variations of the optical phase in response to ultrasound-induced displacement of scatterers. The third mechanism is also based on variations of the optical phase in response to ultrasonic modulation of the index of refraction. As the result of this modulation, the optical phase between two consecutive scattering events is modulated. Multiply scattered light accumulates modulated phase along its paths. An analytical model
was developed by Wang [5]. He calculated the relative contribution of the second and the third mechanism to the modulation of the transmitted light. He also developed a Monte Carlo model based on these two mechanisms [2]. The analytical model was extended by Sakadzic and Wang [6] to anisotropical scattering medium. Monte Carlo Simulation was also used to calculate the interaction of diffuse photon density waves with ultrasound [7].

From a theoretical point of view, describing light propagation in a scattering medium demands solving an integro-differential equation [27]. This transport equation for the radiation can be solved adopting different mathematical models. Among these models, there is a stochastic Monte Carlo model. The Monte Carlo method based on random walk of photons is often used to describe light propagation in scattering media. This simulation method offers a flexible, yet rigorous approach to photon transport in turbid media.

This project presents a novel method, based on Monte Carlo model, to calculate the spatial distribution of the light after interaction with the ultrasound field, in the presence of the optical scatterers. This work has potentially high importance for all researchers working on development
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of the soft biological tissue imaging modality based on acousto–optical effect in turbid medium. The propagation of the light beam through the thin ultrasound slab where thickness is less than one optical transport mean free path resembles realistic situation where light is interacting with the tightly focused ultrasound in biological tissue. We suggest here a modified Monte Carlo model of the ultrasonic modulation of scattered coherent light in a turbid medium. For this purpose only one mechanism of ultrasonic modulation of scattered light was chosen. This mechanism is based on ultrasonic modulation of the index of refraction, which causes a modulation of the optical path lengths between consecutive scattering events.

To calculate the transmitted intensity distribution of scattered light, we use a modified Monte Carlo method similar to that developed by Wang [2]. This method combines the wave properties of light with the particle behavior of propagating photons. The propagation of a light ray is treated as a random walk through the medium. In contrast to the work of Wang [2] we calculate the local intensity on the exit plane as a function of coordinates and not the correlation function integrated over the whole exit plane. Light propagation through the medium was modeled in three dimensions. The incident beam had a Gaussian amplitude distribution, and we also simulated the rectangular amplitude distribution. The intensity distribution of the transmitted light is given by the square of the linear superposition of the various rays that arrive at different incident angles and optical path lengths in each area element in the exit plane.

We developed the modified Monte Carlo method that provides a possibility to detect the component marked by ultrasound field among the diffused transmitted light.
Chapter 1

Light Propagation in a Random Medium

1.1 Introduction

A Random (turbid) medium is a specific state of a medium characterized by the irregular spatial distribution of its physical properties, including optical properties. Such a medium is frequently described as a homogeneous medium containing discrete scattering centers. In a random medium rendering imaging is difficult because of the multiple scattering of light. Scattering of light occurs in the medium with fluctuations of refractive index, those fluctuations can be discrete particles or some continuous variations. Inhomogenities in the medium cause scattering which may alter the direction of propagation, polarization and phase of light. Multiple scattering within a random medium leads to spreading of the light beam and loss of directionality. The propagation of light through such medium may be analyzed either by means of the wave model or the photon model. Photons travel along a straight line until they encounter an inhomogeneity, where they are scattered in a random direction. In a turbid medium made up of random aggregates of scatterers, the photons undergo repeated scattering.
Chapter 1. **Light Propagation in a Random Medium**

The waves in such medium vary randomly in amplitude and phase and must be described in terms of statistical averages and probability densities.

In the theoretical description of light and medium interaction, the medium is treated as a macroscopically homogeneous bulk containing optical scatterers, and is defined by the scattering coefficient, absorption coefficient and anisotropy factor. The characteristics of a single scatterer and some examples are presented in the theoretical works [30], [38]. The study of the characteristics of waves through a random distribution of many particles is well discussed in [27]. When we deal with the light propagation in a medium containing many particles, it is necessary to consider two cases: tenuous and dense distributions.

In the case of the tenuous distribution, when the scatterers locate far from one another, the single scattering approximation is valid. It means, that incident light beam reaches the receiver after encountering very few particles.

As the particle density is increased, we need to take into account attenuation due to scattering and absorption along the path of the wave inside the medium, the multiple scattering effect. Historically, two distinct theories have been developed in dealing with the multiple scattering problem: analytical theory and the transport theory.

In analytical theory the Maxwell equations are considered. This is mathematically rigorous because all the multiple scattering, diffraction and interference effects can be included. In practice it is impossible to obtain a formulation which completely includes all these effects.

A sufficiently rigorous mathematical description of continuous wave light propagation in a scattering medium can be given using the framework of the stationary Radiation Transfer Theory (Transport Theory). In this approach light propagation in a random medium is described by transport of energy by the motion of photons through a medium. The equation of transfer can be solved with help of diffusion approximation. In the diffusion approximation it is assumed, that the diffused intensity encounters
1.2. Optical Properties of Turbid Medium

When light, or electromagnetic radiation in general, propagates through a random medium, the following processes can occur: the light can be scattered or absorbed. These interaction processes are strongly wavelength dependent.

If we want to briefly examine the physical basis for scattering and absorption effects, we can provide the explanation given by Bohren and Huffman in [30]. The following model of light interaction with matter is suggested at the very beginning of the book: "Matter is composed of discrete electrical charges: electrons and protons. If an obstacle, which could be a single electron, an atom or molecule, a solid or liquid particle, is illuminated by an electromagnetic wave, electric charges in the obstacle are set into oscillatory motion by the electric field of the incident wave. Accelerated electric charges radiate electromagnetic energy into all directions; it is this secondary radiation that is called the radiation scattered by the obstacle. In addition to reradiating electromagnetic energy, the excited elementary charges may transform a part of the incident electromagnetic energy into
other forms (thermal energy, for example), a process called absorption." Scattering and absorption are not mutually independent processes, and although, for brevity, we often refer only to scattering, we shall always mean absorption as well."

Absorption and scattering are the two physical phenomena having impact on the light propagation in a turbid medium, that will be discussed in this section. A photon can be absorbed by a molecule if its energy corresponds to the difference in energy between the electronic states of the molecule. Hence, the probability for absorption is strongly wavelength dependent. The energy gained by the medium due to the absorption of light is involved in several processes. It might be re-emitted as fluorescence, contribute to photochemical reactions, or be redistributed among the molecules as heat, inducing a temperature increase. Although both scattering and absorption are important, in this investigation the scattering is the dominant mechanism. Injected photons in medium are likely to be scattered several times before they reach the "detector".

The scattering processes can be divided in two main groups: elastic and inelastic processes. In elastic scattering there is no change of the photon energy, while inelastic scattering results in emission of a photon with an energy different from that of the incident photon. Elastic scattering that occurs when light is scattered by particles with a size much smaller than the wavelength of the light ($\lambda$), for example an atom or a molecule, is called Rayleigh scattering. If the scattering object is too large to be considered as a Rayleigh scatterer, the more complex Mie theory is required to describe the results of the scattering event. Rayleigh scattering theory can be considered as a simplification of the Mie theory in the limit where the size of the particle is negligible to the wavelength of the light. The wavelength dependence of the scattering varies from $\lambda^{-4}$ in the Rayleigh limit to approximately $\lambda^{-2}$ for large particles. This means that the blue light is scattered more strongly than red light, since the latter has a longer wavelength. In the following discussion only the case of elastic scattering is observed.

The optical properties of a single particle are characterized by its absorp-
1.2. Optical Properties of Turbid Medium

tion cross section and scattering cross section. The optical properties of the turbid medium are described by the absorption coefficient, and the scattering coefficient related to the unit of volume [30], [27].

1.2.1 Absorption Coefficient

A relation between the absorption of light in a purely absorbing medium and the thickness of the medium was first determined in 1729 by Bouguer. Some years later Lambert (1760) derived the following mathematical expression

\[
\frac{dI}{I} = \mu_a dx
\]

which describes that each successive layer \( dx \) of the medium absorbs the same fraction \( dI/I \) of the incident intensity \( I \) for a constant \( \mu_a \), that is known as the absorption coefficient with units of inverse length (usually \([cm^{-1}]\)). Therefore, for an incident intensity \( I_0 \) the transmitted intensity \( I \) through a distance \( x \) will be

\[
I = I_0 e^{-\mu_a x}
\]

This relationship known as the Lambert-Bouguer law. The absorption coefficient \( \mu_a \) of the medium depends on the number concentration of particles and their absorption cross sections \( \sigma_a \):

\[
\mu_a = \rho \sigma_a
\]

Consider the total power absorbed by a single particle, that is illuminated by a light wave. Likewise, the energy absorbed inside the particle may by definition be set equal to the energy incident on the area \( \sigma_a \, [cm^2] \).

When the light propagation through a random medium is analyzed by means of the photon model, the probability of survival of a photon after a path–length \( s \) inside the absorbing medium is:

\[
f(s) = \exp(-\mu_a s).
\]
1.2.2 Scattering Coefficient

As already mentioned a turbid medium can be represented as a set of randomly distributed scattering centers. The light beam travels along the straight line until it encounters an inhomogeneity (scattering center) where it is scattered in random directions, fig.1.1. In a turbid medium containing an aggregate of scatterers, the light undergoes repeated scattering.

Consider a single particle, that is illuminated by the optical wave. The total energy scattered in all directions is equal to the energy of the incident wave falling on the area $\sigma_s \ [cm^2]$. Then the scattering coefficient $\mu_s \ [cm^{-1}]$ describes a medium containing many scattering particles at a concentration with a number density $\rho \ [cm^{-3}]$:

$$\mu_s = \rho \sigma_s. \quad (1.5)$$

When the photon propagation in a turbid medium is considered, the path-length $\rho_s = 1/\mu_s$ is the average distance a photon travels between consecu-
1.3. **Scattering Function**

Scattering events (\(\rho_s \,[cm]\) - scattering mean free path). This statement holds provided that the photon path is a straight line between two consequence scattering events in a medium. The probability function for the photon to be scattered at path length \(s\) in a turbid medium is

\[
f(s) = 1 - \exp(-\mu_s s) \quad (1.6)
\]

Derivation of the probability for photon to be scattered at path length \(s\) will be discussed in detail in section 2.

1.3 **Scattering Function**

More substantial information on the angular distribution of the scattered light at a single scattered event is provided by the phase function. The scattering function (phase function) specifies the angular distribution of the scattered light: the amount of light scattered into unit solid angle in a given direction. Let us assume a plane wave \(\vec{E}_i = \vec{E}_0 \exp(ik \cdot \vec{r})\) is incident on the particle. In the far field at a distance \(R \gg d^2/\lambda\), (with \(d\) the dimension of the scatter center and \(\lambda\) the wavelength of the incident light), where interference of waves scattered by different parts of the particle can be neglected, the scattered field is \(\vec{E}_s = \vec{E}_0 \frac{\exp(ikR)}{R} f(\vec{e}, \vec{e}')\). Where \(f(\vec{e}, \vec{e}')\) is the scattering amplitude and describes the amplitude, phase and polarization of the field scattered by the particle in the direction \(\vec{e}'\) when the plane wave being incident from the direction \(\vec{e}\) [27]. The scattering cross section, mentioned above, is related to the scattering amplitude as:

\[
\sigma_s = \int \frac{|f(\vec{e}, \vec{e}')|^2}{4\pi} d\Omega \quad (1.7)
\]

here \(\Omega\) is the solid angle. The scattering cross section describes the total power a particle will scatter at all angles. The phase function:

\[
p(\vec{e}, \vec{e}') = \frac{4\pi}{\sigma_s + \sigma_a} |f(\vec{e}, \vec{e}')|^2 \quad (1.8)
\]

describes the anisotropy of the scattering process.
Chapter 1. Light Propagation in a Random Medium

In the present work the light scattering by a collection of particles (a random medium) is investigated. When a light beam, propagated in a random medium, is incident on a single scatterer along the direction given by the unit vector \( \vec{e} \), it experiences a scattering event. The probability for the light beam to be scattered into the direction \( \vec{e}' \) is given by the phase function \( p(\vec{e}, \vec{e}') \), and it is normalized by the following condition:

\[
\int \frac{4\pi}{p(\vec{e}, \vec{e}')d\Omega = 1}
\]  

(1.9)

The implementation of Monte Carlo method in the studies to of light propagation in a turbid medium requires, among other things a priori knowledge of the scattering phase function. But because of the unknown nature of inhomogeneities in the biological tissues, modeled by turbid medium, the exact function is not known. In some cases it can be measured experimentally, such as for instance in an optically thin tissue. The choice of the phase function is an important feature of any calculation on multiple scattering. Strictly, in a well defined physical problem the phase function is given, not chosen, for instance the phase function for the Mie theory [30]. But it is always possible, without loss of practical accuracy, to approximate the phase function by a simpler one.

From the definition we see that the phase function depends on the scattering angle \( \theta \) and azimuthal angle \( \psi \), see fig. 1.1. It is assumed in the multiple scattering theory that the light propagation through a thick turbid medium depends only on the scattering angle \( \theta \) [38]. By this assumption the scattering is symmetric relative to the direction of the incident wave, and the phase function depends only on the deflection angle \( \theta \) and not on the azimuthal angle \( \psi \), and so \( p(\vec{e}, \vec{e}') = p(\cos \theta) \). Consequently the phase function is the probability density function which defines the probability of the light being scattered between the angles \( \theta \) and \( (\theta + \Delta \theta) \). Such an azimuthal symmetric scattering is a special case, but is generally an accepted approximation used when discussing light scattering in a turbid medium. The most widely used parametric phase function is the Henyey-Greenstein phase function [8], [9]. The use of this phase function in the Monte Carlo method appears to agree well with experiments for most biological media.
Another widely used parameter in multiple light scattering theory is the anisotropy factor:

\[ g = 2\pi \int_{-1}^{1} p(\cos \theta) \cos \theta d(\cos \theta) \] (1.10)

\( g \) is also called the asymmetry parameter, the mean value from the cosine of the deflection angle.

Under the assumption of a azimuthal symmetric scattering the unpolarized phase function can be expanded in series as [38]:

\[ p(\cos \theta) = \sum_{n=0}^{N} \omega_n P_n(\cos \theta) \] (1.11)

were \( P_n(\cos \theta) \) is a Legendre polynomial of order \( n \), and \( N \) is the highest order of the Legendre function occurring in the expansion. The Legendre polynomial constitutes an orthogonal set of functions in \((-1,1)\). The coefficients are given by

\[ \omega_n = \frac{2n + 1}{2} \int_{-1}^{1} p(\cos \theta) P_n(\cos \theta) d(\cos \theta) \] (1.12)

We shall consider some cases of a finite \( N, N = 0; 1; 2 \) and when \( N \) is infinity large.

1) \( N = 0 \), isotropic scattering:

\[ p(\cos \theta) = \frac{1}{4\pi} \] (1.13)

2) \( N = 1 \), linear anisotropic scattering function:

\[ p(\cos \theta) = \frac{1}{4\pi} (1 + 3g \cos \theta) \] (1.14)

The use of such linear anisotropic scattering function is limited because the anisotropy factor has to be \( g < 1/3 \), if one wishes to avoid negative values of the phase function.
Chapter 1.  **Light Propagation in a Random Medium**

3) $N = 2$, the general phase function

$$p(\cos \theta) = \omega_0 + \omega_1 \cos \theta + \omega_2 \frac{1}{2} (3 \cos^2 \theta - 1) \quad (1.15)$$

where $\omega_n$ is obtained from formula (1.12). If set $g = 0$ in (1.10) and use condition (1.9) then from (1.15) the Rayleigh phase function is obtained:

$$p(\cos \theta) = \frac{3}{16\pi} (1 + \cos^2 \theta) \quad (1.16)$$

4) $N = \infty$, for this case in the astronomy literature the Henyey-Greenstein function was introduced:

$$p(\cos \theta) = \frac{1}{4\pi} \frac{1 - g^2}{(1 + g^2 - 2g \cos \theta)^{3/2}}. \quad (1.17)$$

It varies smoothly from isotropic $g = 0$ to a narrow forward peak $g = 1$ or to a narrow backward peak, $g = -1$. At each $g > 0$ the function increases uniformly from the backward direction to the forward direction, see fig.1.2. This makes the function ideal for test calculation on multiple scattering, and the function has been used by many authors [8], [9], [32], [13]. For

![Figure 1.2: Normalized Henyey-Greenstein function $p(\theta)$ in polar coordinates for the different anisotropy factors $g=0.2$, $g=0.5$, $g=0.9$, and Rayleigh phase function where $g=0$.](image)

our simulations, performed using the Monte Carlo model, we choose the
1.3. **Scattering Function**

Henyey-Greenstein (HG) phase function. The reason for choosing the HG phase function is that the scattering angle can be easily calculated. The calculation of the scattering angle for a single scattering event using the Monte Carlo method is discussed in section 3.

To simulate the light propagation in a turbid medium using the Monte Carlo method, one needs to know: scattering coefficient $\mu_s$, absorption coefficient $\mu_a$, anisotropy factor $g$. These properties completely determine a turbid medium where the light suffers multiple scattering.

It is known from literature [24], that most of the biological tissues exhibit scattering with $g > 0.9$ in the near infrared. Similarly it is noted that $\mu_s$ usually is in the range of $5 \text{mm}^{-1}$ to $40 \text{mm}^{-1}$ depending on the density of the specific tissue, and is usually decreases with increasing of the wavelength.

We should point out that for a dense turbid medium, when the propagated light is represented as a photon beam, one more quantity is usually used. It is called the effective diffusion length $\rho^* = 1/(1-g)\mu_s$, after which a photon loses the memory of its initial direction. This length is about $\rho^* = 200 \mu m$ in biological tissues, making it impossible to obtain direct optical images through centimeter thick samples. A 4 cm thick sample with $\rho^* = 200 \mu m$ transmits only $10^{-8}$–$10^{-9}$ of the incoming power [26]. Furthermore, such samples exhibit very low transmission even in the so-called therapeutic window (wavelength of light is $750 – 950 \text{nm}$) where the optical absorption of biological medium is low.
Chapter 1.  Light Propagation in a Random Medium
Chapter 2

Random Variables Sampling

As it is known, the Monte Carlo simulation is a numerical stochastic process, i.e. a sequence of random events. The method is based on sampling of the random variables. To understand this process it is necessary to introduce several definitions from the probability theory.

2.1 Random Variables and their Properties

Definition. A real-valued function $\chi(\omega)$ defined for each outcome $\omega$, in a sample space $\Omega$ is defined to be a random variable. The random variable is discrete if the set of its possible values is finite or countably infinite.

Definition. By means of the Probability function of the random variable $\chi(\omega)$ we define the probability that the random variable $\chi$ with outcome $\omega$ takes on a value $x$.

$$f_\chi(x) = P\{\chi(\omega) = x\}. \quad (2.1)$$

The probability function has the following properties:

$$f_\chi(x) \geq 0, \text{ and } \sum_{\infty} f_\chi(x_i) = 1. \quad (2.2)$$
In these definitions we assume that the random variables belong to a discrete, countable set. Probabilities can be associated with continuous variables as well, giving rise to distribution functions. Such distributions are presented both in nature and in artificial stochastic processes. For example, consider the scattering of a photon by an atom. The angle at which the photon is scattered has values that are continuous between 0° and 180° with some angular intervals occurring more often than others.

We should point out that only for the continuous random variables $\chi(\omega)$ the probability density function exists. For the continuous random variable $\chi(\omega) \in \Omega$ the probability density function satisfies:

$$\int_{\Omega} f_\chi(x) dx = 1. \quad (2.3)$$

The mathematical definition of a continuous probability density function $f(x)$, (pdf) is a function that satisfies the following conditions:

1. The probability that $\chi(\omega) = x$, and $a \leq x \leq b$

$$P\{a \leq \chi(\omega) \leq b\} = P\{a \leq x \leq b\} = \int_{a}^{b} f_\chi(x) dx. \quad (2.4)$$

2. For $\forall x$, $f_\chi(x) \geq 0$, non-negative function

3. If $\chi \in [a, b]$ then $\int_{a}^{b} f_\chi(x) dx = 1.$

Since continuous probability density functions (pdf) are defined for an infinite number of points over a continuous interval, the probability at a single point is always equal to zero. Probabilities are measured over intervals, not single points. That is the area under the curve between two distinct points defines the probability for that interval. This means that the height of the (pdf) can in fact be greater than one.

If the probability density function $f(x)$ for the random variable $x \in [a, b]$ is known the distribution function (cumulative distribution function) should
be defined as
\[ F(x) = \int_{-\infty}^{x} f(x')dx' \]  
(2.5)

For example consider the density function for the well-known uniform random variable \( \xi \in [0, 1] \)
\[ f(\xi) = \begin{cases} 1, & \text{if } 0 < \xi < 1; \\ 0, & \text{otherwise}; \end{cases} \]  
(2.6)

The cumulative distribution function in that case is
\[ F_\xi(\xi) = \begin{cases} 0, & \text{if } \xi \leq 0; \\ \xi, & \text{if } 0 < \xi \leq 1; \\ 1, & \text{if } \xi > 1. \end{cases} \]  
(2.7)

\[ \text{2.2 \ Sampling Random Variables in the Monte Carlo Method} \]

The Monte Carlo method relies on the random sampling of variables from well-defined probability distributions. In doing so, it is usually required that random variables are drawn from the distribution functions that define the process. First we must define what is meant by \textit{sampling}.

We shall start sampling with well known basic random variables \( \xi_1, \xi_2, \ldots \), which are independent and uniformly distributed on \((0, 1)\). It is also assumed that they can be generated by some computer procedure. Such routines are widely available, usually providing satisfactory imitation of truly random variables. We now consider the problem of finding an algorithm to sample the random variables in the Monte Carlo simulation. It is necessary to mention that the general sampling method, usually implied in the Probability Theory, is discussed in the well known book from Kalos [39]. Consider a random variable \( \chi \) defined in the \((a, b)\) interval. In the problem of light propagation in the turbid medium, this variable may be
Figure 2.1: Sampling Random Variables in Monte Carlo Method
2.2. Sampling Random Variables in the Monte Carlo Method

the step-size that a photon will take between photon-medium interaction sites, or the angle of deflection that scattered photon may experience due to a scattering event. There is a normalized probability density function that defines the distribution of $\chi$ over the interval $(a, b)$:

$$\int_a^b f(\chi)d\chi = 1. \quad (2.8)$$

To simulate the photon propagation in a random medium, we wish to be able to choose a value for $\chi$ repeatedly and randomly. We choose for this purpose the random variable, $\xi \in (0, 1)$ which was already mentioned above. The probability density function and the cumulative distribution function are presented by the formulas (2.6) and (2.7). To sample a more generally non-uniformly distributed function $f(\chi)$, we assume there exists a nondecreasing function $\chi = y(\xi)$, which maps $\xi \in (0, 1)$ to $\chi \in (a, b)$. The variable $\chi$ and variable $\xi$ then have a one-to-one mapping and

$$y(\xi) \leq y(\xi_1) \text{ if } \xi \leq \xi_1. \quad (2.9)$$

We can equate the probability that a random variable belongs to some interval $\chi \in (a, \chi_1]$ to the probability that $\xi \in (0, \xi_1]$. We obtain the following [39]:

$$F_\chi(\chi_1) = F_\xi(\xi_1) \quad (2.10)$$

Expanding the cumulative distribution function $F_\chi(\chi_1)$ in terms of the corresponding probability density function (see formula (2.5)) for the left-hand side of the equation, we convert $F_\chi(\chi_1) = F_\xi(\xi_1)$ into:

$$\int_a^{\chi_1} f(\chi)d\chi = \xi_1, \text{ for } \xi_1 \in (0, 1) \quad (2.11)$$

This is the main equation of the sampling process in the Monte Carlo method and is usually used to solve for $\chi_1$ to obtain the function $y(\xi_1)$.

The complete sampling process can be understood from figure 2.1. The key to the Monte Carlo selection of $\chi$ using $\xi$ is to equate the probability that $\xi$ is in the interval $(0, \xi_1]$ with the probability that $\chi$ is in the interval...
Chapter 2. Random Variables Sampling

(0, \chi_1]. From the figure, we are equating the shaded area depicting the integral of \( f(\chi) \) over \((0, \chi_1]\) with the shaded area depicting the integral \( f(\xi) \) over \((0, \xi_1]\). Keep in mind that the total areas under the curves \( f(\chi) \) and \( f(\xi) \) are each equal to unity, as is valid for probability density functions. The whole transformation process \( \chi_1 = y(\xi_1) \) is shown by following the arrows. For each \( \xi_1 \), a \( \chi_1 \) is chosen such that the cumulative distribution functions for \( \xi_1 \) and \( \chi_1 \) provide the same value.

2.2.1 Sampling of a Gaussian Beam Profile

In the following discussion we will treat the example of sampling of Gaussian laser beam profile. In general, laser beam propagation can be approximated by assuming that the laser beam has an ideal Gaussian intensity profile, corresponding to the theoretical TEM\(_{00}\) mode [41].

*Beam profile:* Spatial characteristics describe the distribution of irradiance (radian energy density) across the wave front of an optical beam. The irradiance can be shown as a plot of the relative intensity at the points across a plane that intersects the projected path of the beam.

Here we have to introduce the concept of *irradiance:* at a point on a surface the irradiance \( R \) \([\text{W/cm}^2]\) is a radiant energy flux (or power) incident on an element of the surface, divided by the area of the surface. In other words, the power \( P \) \([\text{W}]\) that irradiates a surface area \( A \) \([\text{cm}^2]\) is called the **Irradiance** \( R \) \([\text{W/cm}^2]\). For a Gaussian beam profile the radiation intensity distribution is characterized by the formula:

\[
R(r) = R_0 \exp\left(-\frac{r^2}{d^2}\right) \quad (2.12)
\]

where \( r = \sqrt{x^2 + y^2} \) is the distance from the beam axis, \( R_0 \) is the intensity in the beam center and \( d \) is the beam size.

The light beam may be described as a photon flux, where the number of photons is proportional to the light intensity. The fluence rate for any irradiation profile may be obtained by launching photons distributed spatially
2.2. Sampling Random Variables in the Monte Carlo Method

with probability density function following the irradiation profile.

The power passing through a circle radius \( r \) equals to

\[
P(r) = R_0 \int_0^r \exp(-\frac{r^2}{d^2})2\pi r\,dr = R_0\pi d^2(1 - \exp(-\frac{r^2}{d^2})) = P_0(1 - \exp(-\frac{r^2}{d^2}))
\]

(2.13)

where \( P_0 \) is the total power in a cross-section of the circle with radius \( r \).

Then the probability of the photon presence inside a circle of radius \( r \) is

\[
P(0 \leq r < \infty) = \frac{P(r)}{P(\infty)} = 1 - \exp(-\frac{r^2}{d^2})
\]

(2.14)

According to the definition of cumulative distribution function we can conclude that distribution function for the Gaussian beam profile is

\[
F(r) = P(0 \leq r < \infty) = 1 - \exp(-\frac{r^2}{d^2})
\]

(2.15)

The probability density function describing the beam profile as a function of radial position \( r \) is

\[
f(r) = \frac{dF}{dr} = \frac{\exp(-\frac{r^2}{d^2})}{\pi d^2}2\pi r = \frac{2r}{d^2}\exp(-\frac{r^2}{d^2}),
\]

(2.16)

where \( \int_0^\infty p(r) = 1. \)

Now we recognize the probability density function for a random number \( \xi \in (0; 1) \) and the corresponding cumulative function \( F(\xi) \) (see formulas (2.6),(2.7)). Equating the two distribution functions \( F(\xi_1) = F(r_1) \), and applying the main equation (2.11) in the sampling process yields to:

\[
\xi_1 = 1 - \exp(-\frac{r_1^2}{d^2}).
\]

(2.17)

Rearrangeing this equation to solve for \( r_1 \) as a function of \( \xi_1 \) we obtain

\[
r_1 = d \sqrt{-\ln(1 - \xi_1)}.
\]

(2.18)

The figure 2.2 illustrates the simulated \( p(r) \) and \( R(r) \) implying the equation \( r = d \sqrt{-\ln(1 - \xi)} \). The dots indicate the histogram for \( p(r) \) and \( R(r) \) created using 10,000 random numbers for \( \xi \). The lines indicate the analytic expression for \( p(r) \) and \( R(r) \).
Chapter 2. Random Variables Sampling

2.2.2 Sampling of Photon’s Step-size $s$

The Monte Carlo model for the light propagation in a turbid medium is based on calculating the photon’s trajectories. It means that for every step of photon propagation in the MC model the step size $s$ between two consequence interaction events of a photon with the medium is calculated. The step size of the photon packet obtained using the sampling of the probability distribution for the photon’s free path $s$, $0 \leq s \leq \infty$. The probability per unit path length of having an interaction is a property of the medium and doesn’t change with the distance the photon has traveled, at least to the point where the medium changes. As a consequence, the probability density function of $s$ behaves exponential [39]:

$$f(s) = \mu_t \exp(-\mu_t s)$$  \hspace{1cm} (2.19)

where $\mu_t$ is the probability per unit length along the photon path for any interaction.

Consider the sampling process of the photon movement with step size $s$. 
2.2. Sampling Random Variables in the Monte Carlo Method

Including this function (2.20) into the main sampling equation (2.11) yields an expression for a sampling value $s_1$ based on the random number $\xi$:

$$\xi = \int_0^{s_1} \mu e^{-\mu s} ds = 1 - e^{-\mu s_1}. \quad (2.20)$$

Solving this for $s_1$:

$$s_1 = -\ln(1 - \xi) \quad \mu \quad (2.21)$$

Which is equivalent to:

$$s_1 = -\ln(\xi_1) \quad \mu \quad , \quad (2.22)$$

where $\xi_1 \in (0; 1)$. 


Chapter 2. Random Variables Sampling
Chapter 3

Monte Carlo Method

3.1 Introduction

The Monte Carlo method is a well known technique that was developed to simulate physical processes using a stochastic model [39]. From a theoretical point of view, the description of light propagation in a scattering medium can be approximated by an integro-differential equation [27]. However, a complete analytical description of this phenomenon is either not available, or very complicated. For light propagation in a random medium, Monte Carlo simulation using a computer is equivalent to finding numerical solutions to the equation of radiative transfer by tracing independent energy packets (photons), each carrying a fraction of the total light energy. The Monte Carlo simulation uses statistical sampling, i.e. sequences of random numbers. The statistical error in the results can be predicted, and generally many trials are needed in order to have a very low statistical error, significantly increasing the computational time. Besides the method provides an approximate solution to the equation of the transport of radiation [8], [27]. The Monte Carlo method can deal with complex geometries in a straightforward manner and allows calculation of multiple physical quantities simultaneously. Several research groups have developed different numerical models based on the Monte Carlo method.
to simulate light propagation in a turbid medium [8], [9], [29],[31], [37]. Research interest in the Monte Carlo model of light propagation in a turbid medium has increased recently because of its flexibility. The Monte Carlo method was also developed to trace the multiple scattered electric field and to simulate the propagation of polarized light in a turbid medium [46], [45].

Prahl and Jacques presented in 1989 the steady-state Monte Carlo method for simulating the light transport in a random medium [8]. The authors have discussed internal reflection of a photon at boundaries, showing how the phase function may be used to generate new scattering angles and suggest a method to estimate the precision of a Monte Carlo simulation. The standard deviations of the mean value were calculated for ten runs of the Monte Carlo program. The comparisons with exact values from van de Hulst’s tables for testing the Monte Carlo implementation were done [8]. In [31] the experimental results are compared with predictions of Monte Carlo computer calculations, to test the numerical modeling of light transport in biological tissues.

L.Wang in [9] proposed a Monte Carlo of steady-state light transport in multi-layered medium. The more general Monte Carlo code to simulate light transport in composite turbid media which can include complex geometric shapes is successfully developed in standard programming language C.

Also the Monte Carlo technique was combined with the diffusion theory by L.Wang, and this approach have been called Hybrid method [32]. Monte Carlo technique is used initially to propagate photons to sufficient depths in the turbid medium where the diffusion theory can be applied with good accuracy. Then the final reflectance is the sum of two reflectances, the first was calculated by Monte Carlo and second is obtained by diffusion theory, taking into account the results from the numerical simulation. The Hybrid method is faster than pure Monte Carlo simulation and more accurate than pure diffusion theory.
One of the problems in light transport within a biological material (random medium) is to provide the spatial distribution of the radiation energy inside or through the turbid medium. In [33], a new method of Monte Carlo simulation is presented, that provides an efficient and direct solution to the spatial distribution of light within the medium. The steady-state results on the propagation of an initially focused laser beam in tissue phantoms and a discussion of their dependence on beam profiles and optical parameters of the tissue are presented in [33].

In [29] the authors investigate the effect of the thin layers of turbid medium on the Monte Carlo simulation results. In this paper, laser light scattering for thin layers has been examined for both the traditional MC and that with new features added and its effect on the reflection, transmission and absorption presented. The authors investigate the steady-state Monte Carlo and suggest also the time resolved MC scheme. For the time resolved analysis, the total optical path length of each photon bundle inside the medium is converted to time of flight $t$, of the photon by using the speed of light in the medium $c$ thus: $t = \frac{L_{\text{total}}}{c}$. The special features are based on the assumption of different absorption coefficient for each thin layer meanwhile the traditional Monte Carlo profile has a continuous photon absorption distribution.

In all papers mentioned above the wave features of the transmitted light such as phase and polarization have not been taken into account. To investigate the propagation of polarized light in a turbid medium the new time-resolved Monte Carlo method was proposed in [42], [43], [44], [45]. The polarization patterns of backscattered light and the spatially distributed polarization states in a birefringent turbid medium are obtained by time-resolved Monte Carlo method in [42]. In [43] the degree of polarization, the transmitted and reflected Mueller matrices were simulated by Monte Carlo method, and the effects of the polarization state of the incident light on the degree of polarization of the transmitted scattered light are investigated. Also the numerical results obtained by the time-resolved Monte Carlo method were compared with the experimentally measured temporal profiles of the Stokes vectors and the degree of polarization [44].
In [45] a single-scattering model as well as the Monte Carlo model of the effect of glucose on polarized light in a turbid medium are presented. In the non-diffusion regime, the two models agree well with each other, but in the diffusion regime the single-scattering model is invalid, but results are predicted by the Monte Carlo method. The Monte Carlo methods were also developed for the optical coherent tomography (OCT). The contribution of the multiple-scattered light to the OCT signal is directly simulated by Monte Carlo technique [34],[35]. The first attempt in Monte Carlo method to trace the multiple scattered electric field through the turbid medium is performed in [46].

The Monte Carlo model where the optical properties of the medium are specified, and the photon trajectory is scored during its propagation in a turbid medium is discussed below. It is necessary to mention that in the sections 3.2 and 3.3 the light transport through the random medium is represented by the propagation of a photon beam as it was done in [8], [9], [29],[31], [37]. Also the rules of photon propagation and the main algorithm of the basic Monte Carlo method are discussed in section 3.2 and 3.3.

We should point out that in the numerical simulation developed in the present work the wave features of the light propagated in a turbid medium are included. The modified Monte Carlo method based on tracing the multiple scattered electric field is used to simulate light transmittance through the medium (Chapter 5). It is necessary to describe the main steps of the basic algorithm. The modified method, is based on the basic algorithm [8] and it is necessary to show the main steps of the method.

3.2 Local Rules of Photon Propagation

For light transport in a turbid medium, the Monte Carlo Model is based on the calculation of the trajectories of propagating photons. The method describes the local rules of the photon propagation expressed as a proba-
3.2. Local Rules of Photon Propagation

bility distributions that describe the path length between two consecutive scattering events, and the angles of deflection in a photon’s trajectory when scattering occurs.

The method is statistical in nature and relies on calculating the propagation of a large number of photons. At first it should be noted, that in the basic Monte Carlo method the light propagating in a turbid medium is represented by a photon beam [8],[9],[32]. It is assumed that photons are neutral ballistic particles and, thus, wave phenomena (coherence and interference) are disregarded. The turbid medium is macroscopically homogeneous, it is assumed that the particle separation is sufficiently large, or the number of particles sufficiently small (single scattering approach).

It was shown in some experimental measurements that the scattering coefficient $\mu_s$ of most biological turbid media in reality is much larger than the absorption coefficient $\mu_a$ [24]. In the numerical model developed in the present project the absorption is neglected. This yields to some differences of the photon tracing from the main algorithm discussed in [8], [9].

To describe the photon propagation in a turbid medium a Cartesian coordinate system is used, and the current position of the photon is specified by coordinates $(x, y, z)$. The current photon direction is specified by a unit vector $\mathbf{r}$, which can be equivalently described by the directional cosines $(\cos X, \cos Y, \cos Z)$. A moving spherical coordinate system, whose $z$ axis is dynamically aligned along the direction of photon propagation is used for the calculation of the changing propagation direction of the photon. In the spherical coordinate system, the deflection angle $\theta$ and the azimuthal angle $\psi$ due to scattering are sampled.

The photon position is initialized to $(0, 0, 0)$ and the directional cosines are set to $(0, 0, 1)$. In order to simulate the fluence rate for some irradiation profiles, photon spatially distribution is launched with probability density function equal to the irradiation profile, for instance Gaussian beam profile.

Once launched, the photon is moving on a distance $s$ where it may be scattered, propagated undisturbed and transmitted out of the medium.
Chapter 3. Monte Carlo Method

The photon is repeatedly moved until it escapes from the medium. The main concept of MC method is to follow the photon path until it experience an interaction. The essential feature here is that photons travel in straight lines until an interaction takes place, so the change in position coordinates can be written down by:

\[ x = x_0 + s \cdot \cos X, \]
\[ y = y_0 + s \cdot \cos Y, \]
\[ z = z_0 + s \cdot \cos Z. \]

(3.1)

The values at the left side (x, y, z) are the new coordinates of photon position and the values at the right side (x_0, y_0, z_0) are the coordinates of the previous photon position, and s is the photon traveling distance in the direction (cos X, cos Y, cos Z).

For every scattering event the Monte Carlo method generates a different step-size s. As shown above, the step-size s must be related to the mean free path-length \( \rho_t \) of a photon in the medium. The mean free path-length \( \rho_t \) is the reciprocal of the attenuation coefficient \( \mu_t \) and in general case \( \mu_t = \mu_s + \mu_a \). We assume that scattering is the dominant effect in our model of light transport through the medium, so we can neglect absorption and simplify: \( \mu_t = \mu_s \). Using the sampling of the probability distribution (see section 2.2.2) we obtain that for each photon propagation step the path-length s is the function of a random variable \( \xi \) uniformly distributed between zero and one:

\[ s = -\frac{\ln(\xi)}{\mu_s} \]

(3.2)

Once the photon has been moved from its initial position, it is ready to get scattered. Now we make use of the Heneye-Greenstein function \( p(\theta) \) (see section 1.3) to describe the photon scattering phenomena, i.e. to calculate the scattering angle \( \theta \). For the photon deflection from its initial trajectory the deflection angle \( \theta \in [0, \pi] \) and an azimuthal angle \( \psi \in [0, 2\pi] \) are generated in the Monte Carlo model, and they are sampled statistically afterwards

\[ \cos \theta = \begin{cases} \frac{1}{2^g} \left[ 1 + g^2 - \left( \frac{1-g^2}{1+g^2} \right)^2 \right], & \text{if } g > 0 \\ 2\xi - 1, & \text{if } g = 0 \end{cases} \]

(3.3)
3.2. Local Rules of Photon Propagation

The anisotropy $g$ equals $< \cos \theta >$, and takes values between $-1$ and $1$.

Next the azimuthal angle $\psi$, which is uniformly distributed over the interval $0$ to $2\pi$, is sampled

$$\psi = 2\pi \xi. \quad (3.4)$$

Once the deflection angle and azimuthal angle are chosen, the new direction of the photon can be calculated (the derivation of this formula is given in [39]):

$$\cos X = \frac{\sin \theta}{\sqrt{(1 - \cos ZZ^2)}} (\cos XX \cos ZZ \cos \psi - \cos YY \sin \psi) + \cos XX \cos \theta,$$

$$\cos Y = \frac{\sin \theta}{\sqrt{(1 - \cos ZZ^2)}} (\cos YY \cos ZZ \cos \psi + \cos XX \sin \psi) + \cos YY \cos \theta,$$

$$\cos Z = - \sin \theta \cos \psi \sqrt{(1 - \cos ZZ^2)} + \cos ZZ \cos \theta \quad (3.5)$$

The old direction cosines are given by $(\cos XX, \cos YY, \cos ZZ)$. The set $(\cos X, \cos Y, \cos Z)$ is not unique, these equations result from a particular choice of the origin of $\psi$ but do satisfy

$$\vec{r} \cdot \vec{r'} = \cos \theta \quad (3.6)$$

$$\cos X^2 + \cos Y^2 + \cos Z^2 = 1 \quad (3.7)$$

If the angle of the photon is too close to normal of the medium surface, $|\cos Z| > 0.99999$, then the following formulas should be used for numerical computations

$$\cos X = \sin \theta \cos \psi,$$

$$\cos Y = \sin \theta \sin \psi,$$

$$\cos Z = \text{SIGN}(\cos ZZ) \cos \theta, \quad (3.8)$$

where $\text{SIGN}(\cos ZZ)$ equals $1$ when $\cos ZZ$ is positive, and $-1$ when $\cos ZZ$ is negative.

As long as we do not consider absorption in our simulations the question has to be raised how the photon should be terminated? In the presented
model the photon can propagate until it crosses a boundary of the turbid medium, where it is scored or killed.

3.3 The Basic Monte Carlo Algorithm

We propose the following algorithm to simulate the local properties of the diffused photon beam by the Monte Carlo method. The turbid medium is confined between the source-plane at the bottom, and the reference–plane at the top and is considered infinite in the other directions. To describe the photon propagation in a turbid medium we select a Cartesian coordinate system with the \((x, y)\) plane assuming to be the source–plane. We choose a photon beam of Gaussian profile of the width \(d\), entering the medium at the coordinate origin. The photon is launched and propagates through the scattering medium until it reaches the reference–plane or source–plane where its position is sampled or where it is removed from calculation (killed). All transmitted photons are collected at the reference-plane. The reference-plane (detector) is divided into cells. The number of cells and their size can be varied for different simulation parameters. The turbid medium used in the Monte Carlo method is fully defined by:

a) the scattering coefficient \(\mu_s [\text{cm}^{-1}]\),

b) the anisotropy factor \(g\),

c) the thickness of the medium (distance between source plane and detector) or other geometrical boundaries.

These parameters remain constant during the whole simulation process. The basic algorithm of Monte Carlo method can now be summarized as following:

1) Launch a photon \((x_0, y_0, z_0)\), from the point of incidence into the medium, in the first step all photons propagate into the same direction.
2) Determine the step-size by \( s = \frac{\ln(\xi)}{\mu_s} \) between two successive scattering events.

3) Move the photon to the new location \((x, y, z)\).

4) If the photon crosses the reference–plane the photon path is terminated, if the photon crosses the source–plane its propagation is also terminated.

5) The calculation of a new direction of the scattered photon is based on the scattering function (the Henyey-Greenstein function).

6) After the calculation of the new propagation direction, we return to steps 2) and 3) to continue the photon propagation.

7) If the photon after \( j \) scattering events crosses the reference–plane (detector) the local coordinates \((x_{\text{detector}}, y_{\text{detector}}, z_{\text{detector}})\) on the detector are sampled:

\[
\begin{align*}
x_{\text{detector}} &= x_j + s_{\text{detector}} \cos X, \\
y_{\text{detector}} &= y_j + s_{\text{detector}} \cos Y, \\
z_{\text{detector}} &= z_j + s_{\text{detector}} \cos Z,
\end{align*}
\]

(3.9)

where \( s_{\text{detector}} \) is the pathlength that the photon runs from the latest \( j \)-scattering event and the point of intersection with the reference plane, where the photon is terminated. Now having finished with this photon, we can launch a new one from step (1). Simulation continues until all photons reach the reference or source planes. Due to multiple scattering only a fraction of all photons reach the reference plane, the rest is excluded from sampling. A part of the diffused photon beam runs over the detector, which has the finite size, or propagates in the back direction and crosses the source plane.

In figure 3.1 we illustrate the typical photon trajectory calculated by MC model for two anisotropy factors. The left figure calculated using anisotropy factor \( g = 0.9 \), and the right figure was obtained for \( g = 0.95 \), all other the optical properties are identical for both figures: \( \mu_s = 10cm^{-1} \), thickness of the medium is \( 1cm \), the cell size is \( 10^{-3}cm \), the photon is launched at
Chapter 3. Monte Carlo Method

Figure 3.1: The typical trajectory of photon in the MC simulation.

Figure 3.2: 1000 photons propagated by the Monte Carlo method.
position $x = 500 \text{ cells}$, $y = 500 \text{ cells}$, $z = 0$. Every photon interaction (scattering) event with the turbid medium is described by red asterisks. From these two pictures we can see how the trajectory of a photon is directly calculated. In the left figure the photon propagation is terminated on the source surface, and the right figure shows a photon moving through the total thickness of the medium.

If the photon number in the simulation increases to $10^3$ photons we obtain figure 3.2. The optical characteristics of the medium are the same as in case of single photon simulation. Here every photon interaction event with the medium is depicted by the red points.
Chapter 3. Monte Carlo Method
Chapter 4

Light diffracted by Sound

The theory of acousto-optics deals with the perturbation of the refractive index caused by sound, and with the propagation of light through this inhomogeneous medium. The refractive index depends on the medium density; consequently, an acoustic wave creates a periodic perturbation of the refractive index. The medium becomes a dynamic graded-index medium - an inhomogeneous medium with time and space varying refractive index. As a result an electromagnetic wave transmitted through the medium is modulated by the sound wave, and scattering and refraction occur. The sound wave acts as a phase grid, moving with sound velocity, its period is equal to the wavelength of the sound wave. If, for example, an optical wave crosses the sound beam perpendicular, the diffracted light will have maxima at angles $\theta_m$ given by

$$\sin \theta_m = m \frac{\lambda}{\Lambda}, \quad m = 0, \pm 1, \pm 2, \pm 3,..$$

(4.1)

where $\lambda$ is the wavelength of the incident light and $\Lambda$ is the wavelength of the sound wave.

The variations of the refractive index of the medium perturbed by the sound are usually very slow compared to the optical period, because the optical frequencies are much higher than those for acoustic waves. As a consequence, it is possible to consider the optical propagation problem
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separately at every instant of time during the relatively slow course of the acoustic cycle, treating the material as a static (frozen) inhomogeneous medium.

On the other hand the phase grid generated by the sound wave moves through the medium with the speed of sound. Because of the Doppler effect there appears a frequency shift in the light diffracted on the moving grid with respect to the incident one [10].

4.1 Sound and the Refractive Index

In the present project only the effect of change of the index of refraction induced by the ultrasound wave is considered. As the propagation velocity of sound is much lower than that of light, we regard the phase grid induced by the sound wave as spatially fixed. The amplitude of this grid depends on the pressure amplitude of the sound wave and the material properties [10], [11]. In presence of a plane sound wave in the medium the following expression holds for the refractive index:

\[ n(y, t) = n_0 - \Delta n_0 \cos(\Omega t - k_s y), \]  

(4.2)

where \( \Delta n_0 = \frac{1}{2} n_0^3 \rho S_0 \), \( n_0 \) is the refractive index of the unperturbed medium, where \( \rho \) is the elastooptic coefficient, \( S_0 \) is the amplitude of density change due to the sound wave see formula (4.42), \( k_s \) is the wave number and \( \Omega \) is the frequency of the sound wave. The derivation of formula (4.2) is shown in Appendix 4.6.

Let us relate the sound wave intensity to the change in the refractive index of the medium. According to [10], the acoustic power is:

\[ P_s = \frac{1}{2} W_s \rho V_s^3 S_0^2 \]  

(4.3)

where \( W_s \) is the cross section area of the acoustic beam, \( \rho \) is the medium density, \( V_s \) is the speed of sound in the medium, \( S_0 \) is the amplitude of the
sound wave. Then it follows
\[ S_0 = \sqrt{\frac{2I_s}{\rho V_s^3}} \]  \hspace{1cm} (4.4)

where \( I_s = P_s/W_s \) is the sound wave intensity. The amplitude of the refractive index modulation by the sound wave is given by
\[ \Delta n_0 = \frac{n_0^3 p}{V_s} \sqrt{\frac{I_s}{2\rho V_s}}. \]  \hspace{1cm} (4.5)

We should point out that intensity here is given in units \( W/m^2 \), the velocity in \( m/s \) and the medium density is in \( kg/m^3 \). For water the refractive index is \( n_0 = 1.33 \) photoelasticity is \( p = 0.31 \), speed of sound in the water is \( V_s = 1.5 \cdot 10^3 m/s \) and the density is \( \rho = 10^3 kg/m^3 \). Using these numbers we obtain \( \Delta n_0 = 2.81 \cdot 10^{-7} \sqrt{I_s} \).

The expression of the permittivity, taking into account the effect of the sound field on the medium can be written as follows
\[ \varepsilon = \varepsilon_0 [1 - \alpha \cos(\Omega t - k_s y)], \]  \hspace{1cm} (4.6)

where \( \varepsilon_0 \) is the unperturbed value of the medium permittivity, and the amplitude of the permittivity modulation equals to
\[ \alpha = 2 \frac{\Delta n}{n_0} = n_0^2 p S_0 = \frac{n_0^2 p}{\rho V_s^3} \sqrt{\frac{2I_s}{\rho V_s}}. \]  \hspace{1cm} (4.7)

For water \( \varepsilon_0 = 1.769, \alpha = 4.22 \cdot 10^{-7} \sqrt{I_s} [\sqrt{m^3/kg}] \). Thus, the perturbation of the refractive index and the permittivity due to the sound wave depend essentially on the sound wave intensity.

### 4.2 Mathematical Model of the Problem

The rigorous theory of light and sound interaction is based on the solution of the general wave equations obtained from the set of Maxwell equations.
The wave equation for the non-magnetic, non-conducting medium is:

$$\nabla^2 E(x, y, z, t) = \frac{1}{c^2} \frac{\delta^2}{\delta t^2} (\varepsilon E)$$

(4.8)

Here $E$ is a component of the electric field and $\varepsilon$ is the permittivity of the medium.

Let us consider a plane electromagnetic wave incident on the $z = 0$ plane at an angle $\theta$.

$$E = E_0 \exp[j(k_0 y + k_0 z - \omega_0 t)]$$

(4.9)

where $E_0$ is the amplitude of the incident wave, $\omega$ its frequency, $k_{0x} = 0$, $k_{0y} = k_0 \sin \theta$, $k_{0z} = k_0 \cos \theta$ are the projections of the wave vector on the coordinate axes, $k_0 = \frac{\omega_0}{c} n_0$ is the optical wave number, and $n_0$ is the refractive index of the unperturbed medium.

The sound wave propagates in the $y$ direction and fills the region between the two planes $z = 0$ and $z = w$. For the given geometry it is assumed (from the symmetry of the problem) that none of the fields depend on $x$ coordinate. Therefore the wave equation for the light wave in the region of the light and sound interaction ($0 \leq z \leq w$) can be written as

$$\frac{\delta^2 E}{\delta y^2} + \frac{\delta^2 E}{\delta z^2} = \frac{1}{c^2} \frac{\delta^2}{\delta t^2} (\varepsilon E)$$

(4.10)

where $\varepsilon \approx n^2 \approx n_0^2 - 2n_0 \Delta n_0 \cos(k_y y - \Omega t)$, $k_y = \frac{2\pi}{\Lambda}$, $\Lambda$, $\Omega$ are the wave number, wavelength and frequency of the sound wave inside the medium.

If the incident angle of the light beam is small and $\lambda << \Lambda$, the solution of the given equation can be expanded in series (as developed in [10]):

$$E(y, z, t) = \exp[j(k_0 y + k_0 z) - \omega_0 t] \sum_{-\infty}^{\infty} V_m(z) \exp[jm(k_y y - \Omega t)]$$

(4.11)

Without solving the wave equation, we should mention some of the features of such a superposition of the scattered waves. Frequencies of these waves are $\omega_m = \omega_0 + m\Omega$, ($m = 0, \pm 1, \pm 2...$). Since the frequency of the sound wave, on which the light diffraction occurs, is much smaller then
4.2. Mathematical Model of the Problem

the light frequency \((\Omega \ll \omega_0)\), the frequencies \(\omega_m \approx \omega_0\). The absolute values of the wave vectors \(k_m\) of the scattered waves are approximately the same as for the incident light wave

\[
k_m = \frac{\omega_0 + m\Omega}{c} n_0 \approx k_0.
\] (4.12)

where \(k_0\) is the wave number of the incident light wave on the sound field.

The projections of the wave vector \(k_m\) on the \(x\)-axis satisfy the conditions \(k_{mx} = k_0x\) and \(k_{my} = k_0 \sin \theta + mk_s\). The projection of the wave vector \(k_m\) on the \(z\) axis, in the approximation used here, doesn’t change and remains equal to \(k_{mz} = k_0 \cos \theta\). Therefore the angle \(\theta_m\) between the vector \(k_m\) and the \(z\)-axis is determined by the ratio:

\[
\sin \theta_m = \frac{k_{my}}{k_m} \approx \sin \theta_0 + m \frac{k_s}{k_0} = \sin \theta_0 + m \frac{\lambda_0}{n_0 \Lambda}
\] (4.13)

The substitution of expansion (4.11) in equation (4.10) allows to obtain the differential equations in a form of the recurrence relations to estimate the amplitudes \(V_m(z)\):

\[
\frac{d^2 V_m}{dz^2} + 2jk_0 \cos \theta \frac{dV_m}{dz} - mk_s(2k_0 \sin \theta + mk_s)V_m = -\frac{k_0^2 \Delta n_0}{n_0}(V_{m+1} + V_{m-1})
\] (4.14)

Under the assumption that the functions \(V_m(z)\) vary sufficiently slow in the region \(0 \leq z \leq w\), the system of differential equations of the first order can be obtained [10]:

\[
\frac{dV_m}{dz} + j \mu_m V_m = j \frac{k_0 \Delta n_0}{2n_0 \cos \theta} (V_{m+1} + V_{m-1}),
\] (4.15)

where

\[
\mu_m = \frac{mk_s(2k_0 \sin \theta + mk_s)}{2k_0 \cos \theta}.
\] (4.16)

The intensity of the \(m\)-diffraction order \(I_m\) is determined by the ratio \(I_m = V_m V_m^*\). The solution of these equations is usually obtained with some additional limitations. Under the ordinary diffraction conditions the amplitude of the waves reflected by the sound field can be neglected [11].

It is obvious, that the characteristics of the diffracted light beams, such as the direction in the space and intensity, depend on the properties of
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the sound field (frequency, intensity, thickness of the sound field), and also depend on the angle $\theta$. Moreover, because of the Doppler effect, the frequency of the light diffracted on the moving grid is shifted from the initial value by the magnitude of the sound frequency.

4.3 Limiting Cases

Physically, the light scattering on the sound wave can be understood as the diffraction of light on the phase grid moving with the speed of sound. The nature of the diffraction essentially depends on the dimensions of the light and sound interaction area, in other words, on the thickness $w$ of the sound field.

For a small width $w$ of the sound beam, the diffraction grid can be treated as a plane phase grid. The directions of the diffraction maxima are detected by formula (4.13) similarly to the simple diffraction phase grid [40]. The diffraction pattern consists of the set of diffraction maxima, located symmetrically relative to the direction of the incident light. This type of diffraction is called Raman–Natt diffraction. It occurs at all angles between the incident light and the sound field.

Fundamentally different effects appear for the light diffraction on the sound field when the thickness of the sound beam is large. In this case the diffraction grating is three-dimensional. The nature of the light diffraction on the sound beam with large $w$ is similar to the diffraction of X-rays on the crystal structure. Such diffraction occurs only for some certain incident angles, namely, the angle must satisfy the Bragg condition:

$$\sin \theta_B = \frac{\lambda_0}{2n_0\Lambda}$$  \hspace{1cm} (4.17)

This diffraction regime is called the Bragg diffraction. The presence of only one diffracted maximum is typical for this regime.

The criterion of transition between the Raman–Natt and Bragg diffraction
4.3. Limiting Cases

regimes is related to the growing importance of the phase correlations between all the scattered waves in the system when the length of the interaction area is increased.

The plane grid approximation assumes that at the end of the interaction area the phase increment equals to $k_0 w$, but in reality for the scattered ray it equals to $k_0 w \cos \theta_m$. For angles $\theta_m << 1$ the difference

$$k_0 w (1 - \cos \theta_m) \approx w \frac{k_s^2}{2k_0} m^2,$$

(4.18)

and is getting smaller with decreasing of sound beam widths and increasing of the sound wavelength. Here $k_s$ is the wave number of the sound wave, $k_0$ - is the wave number of the light wave in the medium. The magnitude:

$$Q = \frac{k_s^2}{k_0} w = \frac{2\pi \lambda_0}{n_0 \Lambda^2} w$$

(4.19)

is called Klein-Cook parameter for the light diffraction on the sound wave and determines the dominant diffraction regime [10], [11]. If the condition

$$\frac{2\pi \lambda_0 w}{n_0 \Lambda^2} << 1,$$

(4.20)

is satisfied, Raman-Natt diffraction takes place. The power of the incident radiation is distributed among the set of the diffraction orders symmetrically relative to the transmitted light. When the parameters of the sound wave satisfy the condition

$$\frac{2\pi \lambda_0 w}{n_0 \Lambda^2} >> 1,$$

(4.21)

then the Bragg diffraction on the sound wave dominates. It occurs only if the light falls on the sound beam at the Bragg angle:

$$\theta_B = \arcsin \frac{1}{2} \frac{\lambda_0}{n_0 \Lambda}$$

(4.22)

In this case the light deflection occurs only in the first diffraction order $+1$st and the diffracted light emerges from the sound beam under the Bragg angle.
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4.4 Raman-Nath Diffraction Regime

In this section the simplest physical model of light diffraction on a sound wave, Raman-Nath diffraction is considered. We restrict ourselves to the case where the direction of the incident optical wave is perpendicular to the propagation of the sound wave. In this case the electric field \( E(y,z,t) \) can be written as follows:

\[
E(y,z,t) = E_0 \exp[j(k_0z - \omega_0t)] ,
\]

where \( E_0 \) is the amplitude of the incident wave, \( \omega_0 \) is the frequency of the light wave, \( k_0 = kn = \frac{2\pi}{\lambda_0} \) is the wave number, and \( n \) is the refractive index of the medium. Taking into account the modulation by the sound wave, we express the optical wave in the form:

\[
E(y,z,t) = E_0 \exp[jkz(n_0 + \Delta n_0 \cos(k_s y - \Omega t)) - j\omega_0t] \tag{4.24}
\]

Obviously, in the present situation the light and sound interaction leads to a pure phase modulation of the light. This equation can be written as:

\[
E = E_0 \exp[jkz(n_0 + \Delta n_0 \cos(k_s y - \Omega t))] - j\omega_0t] \tag{4.25}
\]

where the following notations are used: \( \nu(z) = 2\pi\Delta n_0 z/\lambda_0, \phi_s = k_s y - \Omega t \). The second exponent can be expanded in series, and that:

\[
e^{j\nu \cos \phi_s} = \sum C_m(\nu)e^{jm\phi_s}, m = 0, \pm 1, \pm 2, ...
\]

The expansion coefficients are obtained using the well-known formulas:

\[
C_m(\nu) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{j(\nu \cos \phi_s - m\phi_s)} d\phi_s \tag{4.27}
\]

After the integration we obtain the following result:

\[
C_m(\nu) = (-j)^m J_m(\nu), \tag{4.28}
\]

where \( J_m(\nu) \) is the the \( m \)-th order Bessel function of the first kind. Finally, the electric field of the optical wave in the region \( 0 < z < w \) is obtained:

\[
E(y,z,t) = E_0 \exp[j(kn_0z - \omega_0t)] \sum_{-\infty}^{\infty} (-j)^m J_m(\nu) \exp[jm(k_s y - \Omega t)]. \tag{4.29}
\]
4.4. Raman-Nath Diffraction Regime

The same expression for the electric field can be obtained solving the set of equations (4.15), if angle $\theta_0 = 0$, and if is assumed that the value $\mu_m \to 0$. Then from formula (4.16) we obtain:

$$\frac{m^2 k_s^2 w}{2k_0} \to 0,$$

(4.30)

or, in other word $Q \to 0$, here $k_0 = \frac{2\pi n_0}{\lambda_0}$.

As a result of electromagnetic and sound wave interaction the set of diffraction maxima appears, similar to a phase grating. The diffracted waves make the angle $\theta_m$ with the $z$-axis, and the condition:

$$\sin \theta_m = \frac{\lambda_0}{n_0 \Lambda} m$$

(4.31)

is satisfied. At the same time, the frequency of the waves scattered at angle $\theta_m$, due to the Doppler shift becomes equal to $\omega_m = \omega_0 + \Delta \omega$. Most easily the Doppler shift can be understood as follows: an observer looking at the $m$th order sees the sound-induced radiating dipoles moving upward with sound velocity $V$. The velocity component in the scattering direction is given by $V \sin \theta_m$, we find for the Doppler shift

$$\Delta \omega = \frac{\omega}{c} V \sin \theta_m = k_0 \frac{\Omega}{k_s} \sin \theta_m;$$

(4.32)

From another side, if we use the formula (4.31), then $\Delta \omega = m \Omega$.

The light intensity of the $m$th diffraction maximum is defined by calculating $EE^*$. After passing the distance $z$ the intensity distribution of the light at the diffraction maxima can be described by formula

$$I_m = I_0 f_m^2(\nu),$$

(4.33)

where $I_0$ is the intensity of the incident light, $I_m$ is the light intensity in the $m$th diffraction maximum and $\nu(z) = 2\pi \Delta n_0 z / \lambda_0$. Figure 4.1 shows the intensity of orders $I_m / I_0 = f_m^2(\nu)$, diffracted by a thin sound column, as a function of the peak phase delay $\nu$. If the parameter $\nu$ is such that $\nu << 1$, the first-order diffraction peak has an amplitude proportional to $\nu$, and the $m$-th order peak has an amplitude proportional to $\nu^m$. For
larger ν, the amplitude of the zeroth-order peak decreases equal to 0 at
ν = 2.405, while the amplitude of the first-order peak reaches maximum
when ν = 1.84. When ν is sufficiently large, we see many diffraction
peaks, sometimes 20 or even more. When ν → 0, using the approximate
expression for Bessel function with small argument, we readily find that
only three orders (−1, 0, +1) remain. This is the so-called limit of weak
interaction.

4.5 Bragg Diffraction Regime

In isotropic media with increasing as the length of the optoacoustic inter-
action, the distortion of the optical beam takes place inside the interaction
area. Therefore, it is important to take into account the phase relations
between waves from the different diffraction maxima. If Q >> 1 the ob-
servable diffraction doesn’t occur at an arbitrary incident angle θ₀ of the
light. And only at specific incident angles θ₀, close to Bragg angle θ_B, the
4.5. Bragg Diffraction Regime

effective diffraction occurs in +1st or −1st diffraction order. Therefore in
the system of equations (4.15) it is possible to reserve components with
$m = 0$ and $m = 1$, or $m = 0$ and $m = −1$. Let us consider the $m = 0$ and
$m = 1$ components. In this case the system of equations (4.15) transforms
to system of two equations:

$$
\begin{align*}
\frac{dV_1}{dz} + j\mu_1 V_1 &= jaV_0 \\
\frac{dV_0}{dz} &= jaV_1
\end{align*}
$$

(4.34)

where

$$
\mu_1 = \frac{2k_0k_0 \sin \theta_0 + k_2^2}{2k_0 \cos \theta_0}
$$

(4.35)

$$
a = \frac{k_0 \Delta n_0}{2n_0 \cos \theta_0}.
$$

The solution of this system, considering the boundary conditions $V_0(0) = E_0$, $V_1(0) = 0$, is follows:

$$
V_0(z) = \frac{E_0}{\sqrt{\mu_1^2 + 4a^2}} (\alpha_1e^{j\alpha_2z} - \alpha_2e^{j\alpha_1z})
$$

(4.36)

$$
V_1(z) = \frac{E_0}{\sqrt{\mu_1^2 + 4a^2}} (e^{j\alpha_2z} - e^{j\alpha_1z})
$$

where

$$
\alpha_{1,2} = \frac{-\mu_1^2 \pm \sqrt{\mu_1^2 + 4a^2}}{2}
$$

(4.37)

The light intensity of the diffracted light depended on coordinate $z$ is:

$$
I_0 = V_0V_0^* = \frac{E_0^2}{\mu_1^2 + 4a^2} \left[ \mu_1^2 + 4a^2 \cos^2 \left( \frac{\sqrt{\mu_1^2 + 4a^2}}{2}z \right) \right]
$$

(4.38)

$$
I_1 = V_1V_1^* = \frac{4E_0^2a^2}{\mu_1^2 + 4a^2} \sin^2 \left( \frac{\sqrt{\mu_1^2 + 4a^2}}{2}z \right)
$$
When $\mu_1 = 0$ in the formula (4.35) then $\sin \theta_0 = -\frac{k_i}{2k_0} = -\sin \theta_B$, which exactly equals to Bragg condition. For this case

$$I_0 = E_0^2 \cos^2(az),$$

(4.39)

and

$$I_1 = E_0^2 \sin^2(az).$$

(4.40)

where

$$a = \frac{k_0 \Delta n_0}{2n_0 \cos \theta_0}$$

(4.41)

Figure 4.2 shows the intensity of orders $I_0$ and $I_1$, as a function of the parameter $\nu/2$ where $\nu = 2\pi \Delta n_0 z / \lambda_0$. Here its assumed that angle $\theta_0$ is small and $\cos \theta_0 \to 1$ so $a = \nu/2$.

Figure 4.2: The intensities of orders $I_m$, $m = 0, 1$ as functions of parameter $\nu/2$, $I_i$ is the intensity of the incident light.
4.6 Appendix

The sound field can be represented by the symbol $S$ that is taken to denote fractional density change in a liquid. If the plane sound wave travels along the $y$–axis, then it can be suggested that

$$S(y, t) = S_0 \cos(\Omega t - k_s y), \quad (4.42)$$

where $S_0$ is the amplitude and $\Omega$ is the frequency of the sound wave, $k_s$ is its wave vector (wave number). In the isotropic medium concentration of particles, molecules and atoms becomes dependent on the space coordinates and time. In the case of small deformations the particle (molecules) concentration can be written as follows:

$$N(y, t) = N_0 [1 - S(y, t)], \quad (4.43)$$

where $N_0$ is the equilibrium concentration of the molecules in the medium. For the gases the Lorenz-Lorenz formula is valid, relating the permittivity of the medium with the number of polarized particles in a unit volume $N$

$$\frac{\varepsilon - 1}{\varepsilon + 2} \cdot \frac{1}{N(y, t)} = \text{const.} \quad (4.44)$$

Now it can be easily seen that

$$\Delta \varepsilon = \frac{(\varepsilon - 1)(\varepsilon + 2)}{3} \cdot \frac{\Delta N}{N}. \quad (4.45)$$

For the weak deformations one can write

$$\frac{\Delta N}{N} \approx -S \quad (4.46)$$

So that the relative change in the refractive index of the medium is proportional to the medium deformation

$$\frac{\Delta \varepsilon}{\varepsilon} = -\frac{(\varepsilon - 1)(\varepsilon + 2)}{3\varepsilon}S. \quad (4.47)$$

The alteration of the medium permittivity due to the deformation is called photo–elastic effect. Generally when considering the photo–elastic effect,
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the relation between changes of the medium’s permittivity with the deformation is described by formula:

$$\Delta \left( \frac{1}{\varepsilon} \right) = p \cdot S,$$

(4.48)

where $p$ is the elastooptic coefficient. It is an easy matter to obtain the following expression

$$\frac{\Delta \varepsilon}{\varepsilon} = -\varepsilon p S$$

(4.49)

When this result is compared with the one for $\Delta \varepsilon / \varepsilon$ obtained using the Lorenz-Lorenz formula, we can obtain the following expression for the photoelasticity constant

$$p = -\frac{(\varepsilon - 1)(\varepsilon + 2)}{3\varepsilon^2}.$$  

(4.50)

For water $\varepsilon = 1.769$ and then the value $p = 0.31$ calculated from the formula above coincides with experimental one.

Taking into account, that the refractive index $n^2 = \varepsilon$, we have

$$\frac{2\Delta n}{n} = \frac{\Delta \varepsilon}{\varepsilon} = -\varepsilon p S = -n^2 p S,$$

(4.51)

and therefore:

$$\Delta n = -\frac{1}{2} n^3 p S,$$

(4.52)

And finally the following expression holds for the refractive index

$$n(y, t) = n_0 - \Delta n_0 \cos(\Omega t - k_s y),$$

(4.53)

where $\Delta n_0 = \frac{1}{2} n_0^3 p S_0$, $n_0$ is the refractive index of the unperturbed medium.
Chapter 5

Numerical Experiment

5.1 Introduction

An advanced novel method to calculate the spatial distribution of the light after interaction with the ultrasound field, in the presence of the optical scatterers, is presented here. The propagation of a light beam through a thin ultrasound slab realistically represents the interaction of light with a tightly focused ultrasound beam in biological tissue. We consider here an ultrasonic modulation of the coherent light in presence of optical scatterers in a medium when absorption is neglected. For this purpose only one mechanism of the ultrasonic modulation of scattered light is considered. This mechanism is based on ultrasonic modulation of the refractive index, which causes a modulation of the optical path lengths between consecutive scattering events. Basically, we use the Monte Carlo method to simulate the light propagation but the phase information is also added to the wave packets. The final goal of this project is to develop a theoretical (Monte Carlo) model of the propagation of frequency marked photons in a turbid medium and to analyze its detectability.

The local intensity in the exit plane as a function of the position is obtained by the modified Monte Carlo method in the present chapter. The intensity
distribution of the transmitted light is given by the square of the linear superposition of the rays arriving with different incident angles and optical path lengths on each surface element in the exit plane. This section presents the results of the numerical simulations (numerical experiments). Every run of the Monte Carlo program yields the intensity distribution of the "sound"-modulated light on the detector (exit) plane. The numerical experiments are performed in several steps: at first we simulate the phase modulation of the light scattered only in the sound field, then we add optical scatterers in the whole turbid medium. With the greater flexibility of the modified Monte Carlo method, it is shown that the new model serves well as a numerical phantom to substitute the otherwise expensive experiments.

5.2 Formulation of the Problem

The modified Monte Carlo method for the problem is illustrated in figure 5.1. The investigated medium is confined between the source plane at the bottom, and the reference plane at the top and is considered infinite in the other directions. The light beam enters the medium at the coordinate origin \((0, 0, 0)\) and has a Gaussian beam profile of width \(d\). The acoustic wave propagates through the medium along the \(y\) direction with the wavelength \(\Lambda\), and wave vector \(\vec{k}_s\). The wavelength of the light beam is \(\lambda_0\), the light beam enters the turbid medium with an angle \(\phi\) with respect to the \(z\) axis. The plane sound wave is represented by a refractive index periodically varying in space:

\[
n(y) = n_0 + \Delta n \cos \left(\frac{2\pi}{\Lambda} y\right), \tag{5.1}\]

where \(n_0\) is the refractive index of the unperturbed medium, \(\Delta n\) is the amplitude of refractive index oscillations induced by the sound wave. All transmitted light is collected at the reference–plane (detector). Using the Monte Carlo method the local intensity in the detector plane is calculated as function of position. We carry out the numerical experiments in several steps: first we deal with the simplest model when the optical scatterers
Modified Monte Carlo Method

Figure 5.1: The geometry of the numerical experiment.

($g < 1$) are present only in the sound-field, inside the layer $[z_u, z_u + w]$ (see figure (5.1)). The medium in the region infront of and behind the sound-field is treated as a "clear" medium, $g = 1$. In the next step we assume that the medium outside of the sound-field is turbid and scatters light. Scattering outside of the sound wave would mainly add some noise. Qualitatively, we do not expect much influence of scattering processes outside of the sound field.

5.3 Modified Monte Carlo Method

To calculate the intensity distribution of the transmitted scattered light, we use the modified Monte Carlo method. This method combines the wave properties of light with the particle behavior of propagating photons. The intensity distribution of transmitted light is given by the square of the linear superposition of the amplitude of the electric field of various rays arriving with different incident angles and optical path lengths in each surface element in the exit plane. It is assumed that the amplitude of each ray is not changed during its propagation.

We should point out that incorporation of the phase information into the Monte Carlo technique was first reported in [14], who used this technique.
Chapter 5. Numerical Experiment

to simulate the diffraction effects of a focused beam in two-photon microscopy. The authors compare the results from the modified Monte Carlo method with the Huygens-Fresnel principle and achieve good agreement. In our model the propagating light is represented by a number of rays with a random walk through the medium. The polarization and amplitudes remain constant.

The modified Monte Carlo method of the problem is illustrated in figure (5.1) and presented in the following section. An acoustic wave propagates through the medium along the \( y \) direction with the wavelength \( \Lambda \). The wavelength of the light beam is \( \lambda_0 \), the light beam enters the turbid medium with an angle \( \phi \) with respect to the \( z \) axis. This means that all the rays are launched into the medium with the angle \( \phi \). In addition, the phase of the rays are adjusted so that all rays are members of a plane wave entering the medium at an angle \( \phi \). As a first step, we assume that \( g < 1 \) only in the infinitely wide layer \([z_u, z_u + w]\) where the refractive index changes periodically (see figure 5.1). The propagation of the ray in such medium in the framework of the modified Monte Carlo method can be described by the following steps:

1) Launch a ray at \((x_0, y_0, z_0),(0, 0, 0)\).

2) Move the ray to a new location \((x, y, z)\) with \( g = 1 \), until it reaches the layer \([z_u, z_u + w]\) with the periodic modulation of refraction index. Each section contributes to the total phase as

\[
\varphi_j = \frac{2\pi}{\lambda_0 n_0 s_j},
\]  

(5.2)

where \( s_j \) is the \( j \)-th free path and, \( n_0 \) is the refraction index of the unperturbed medium.

3) If the ray is found inside the layer \([z_u, z_u + w]\), then \( g < 1 \) and the scattering process is simulated by calculating the deflection angle \( \theta_j \). The phase variation induced by the modulation of refraction index along the
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The *j*th free path is

\[
\varphi_j(\vec{r}_j) = k_0 \int_{0}^{s_j} n(\vec{r}_j, \alpha_j, s) \, ds, \tag{5.3}
\]

where \( \vec{r}_j \) is the position-vector of the *j*th scattering event, \( s_j \) is the path length between \( j-1 \) and *j* scattering events, \( \alpha_j \) is the angle between the direction of the sound wave and the direction of the ray propagation.

4) The position of the next scattering event is generated, and we return to the step (2). If the ray is outside the layer, then the anisotropy factor \( g \) is set equal to 1. The ray effectively propagates without scattering until it reaches the detector plane.

After calculating the propagation of all rays, the intensity is obtained as \( I \sim EE^* \), where \( E = \sum_{n=1}^{N} \exp(j\varphi_n) \) is the sum of all *N* rays in the cell. Where \( \varphi_n \) is the phase of the *n*th ray, obtained as \( \varphi_n = \sum \varphi_j \), here \( \varphi_j \) is calculated in step (2). The far-field intensity distribution is obtained at the detector plane. In our simulation the detector plane consists of about 500x500 cells, and the typical cell size is 10^{-3} cm.

The modified Monte Carlo method allows us to investigate the ultrasonic modulation of scattered light in a turbid medium with various physical properties, different scattering coefficients and anisotropy factors. In our simulations the anisotropy factor has values in the range 0.86 \( \leq g \leq 0.99 \), and the scattering coefficient is within the 1cm^{-1} < \( \mu_s < 5cm^{-1} \) range. An important property of the modified Monte Carlo method is the amount of the rays launched in the medium. The Monte Carlo method is a statistical method and is based on sampling of a large number of rays. However the computational time grows linearly as the number of the sampled rays is increased.

In the next sections 5.4–5.6 we investigate the case, when the optical scattering take place only in the sound-field \( (g < 1) \), inside the layer \([z_u, z_u + w] \) (see figure (5.1)). Absorption is neglected completely. The medium in the regions infront and behind the sound-field is treated as a "clear" medium with \( g = 1 \).
5.4 The Light Beam Perpendicular Incidents on the Sound Field

If the light beam crosses the plane sound wave (see figure 5.1) orthogonally, all parameters are adjusted so that \( Q < 1, \) \( Q = 2\pi\lambda_0 w/n_0\Lambda^2 \) and we have the light diffraction on a phase-grid, we are in the Raman-Nath diffraction regime (see section 4). The numerical experiment is carried out with the following conditions:

1) The turbid medium has the following optical properties: \( g = 0.99, \) \( \mu_s = 5cm^{-1}. \)

2) The thickness of the sound field is \( w = 0.1cm, \) the distance to the detector-plane is \( a = 11cm, \) and the distance to the sound field is \( z_u = 1cm. \)

3) Optical scatterers (\( g < 1) \) are present only in the sound–field, inside the layer \([z_u; z_u + w].\)

4) The wavelength of the incident light is \( \lambda_0 = 532 \cdot 10^{-7}cm, \) the width of the light beam is \( d = 10^{-2}cm. \)

5) The sound wave has a wavelength of \( \Lambda = 5.7 \cdot 10^{-3}cm \) in the medium.

6) The light beam is orthogonal to the layer \([z_u, z_u + w]\) with the periodic modulation of the refractive index, the photon beam enters the medium at the point \( x = 250 \) cells, \( y = 250 \) cells, see figure(5.1,left). The refractive index of the unperturbed medium is \( n_0 = 1.33. \)

When the paths of all rays are calculated by the modified Monte Carlo method, the intensity distribution is obtained at the detector–plane. The intensity is calculated as \( I \sim EE^*, \) where \( E = \sum_{n=1}^{N} \exp(j\varphi_n) \) is the sum of all \( N \) rays in the cell.

First we investigated the simplest case, by setting the amplitude of the refractive index modulation \( \Delta n = 0.0, \) figure 5.2. There is no phase modulation in the layer \([z_u, z_u + w]\) and only scattering is presented in this region.
5.4. The Light Beam Perpendicular Incidents on the Sound Field

$g < 1$, figure 5.1, (left). In the next step the phase modulation is introduced with $\Delta n = 10^{-5}$ and we obtain the results shown on the right side in figure (5.2). The physical interpretation of the intensity distribution shown in figure (5.2) is that the plane sound wave propagating through a medium diffracts the light beam much in the same way as a diffraction grating does. And the position of each diffraction maximum can be calculated by the formula

$$\sin \theta_m = m \frac{\lambda_0}{n_0 \Lambda},$$

(5.4)

where $m = 1, 2, \ldots$.

Figure 5.3 shows the intensity distribution for different amplitudes of the refractive index modulation. For each amplitude of the refractive index $\Delta n$ we see the evolution in the simulation results, the number of the diffracted peaks increases with growing $\Delta n$. If we decrease $\Delta n$ so that $\Delta n = 10^{-5}$, and all others characteristics of the experiment are kept constant then we receive only two additional maxima at positions symmetric relatively to the main maximum (see figure 5.3). As in the previous case, the ultrasound wave generates a phase grid, and under the conditions of weak interaction [10], [11] the transmitted light generates only two first order maxima on each side of the un-deflected beam, the zero-order maximum.

The results in figure 5.3 suggest that the number of the diffraction maxima depend on $\Delta n$, in other words on the power of the sound field. With increasing power and constant factor $Q = 2\pi \lambda_0 w / n_0 \Lambda^2 < 1$, the number of diffraction maxima increase. Simultaneously, the energy is distributed between adjacent diffraction maxima as it is given by equation (4.29). It is interesting to note that the condition of energy conservation (the waves refracted in the opposite direction are neglected) leads to well known relation of the Bessel function of the first kind

$$j_0^2 + 2(j_1^2 + j_2^2 + \ldots + j_m^2 + \ldots) = 1.$$  

(5.5)

This condition allows to estimate with some accuracy the number of the peaks in the Raman–Nath diffraction regime for a given width and power of the sound field. The Bessel function argument is $\nu = 2\pi \Delta n w / \lambda_0$. For the
width \( w = 0.1 \text{cm} \), \( \Delta n = 10^{-4} \) and the argument value \( \nu = 1.181 \), it can be easily checked that relation

\[
J_0^2(\nu) + 2(J_1^2(\nu) + J_2^2(\nu)) \approx 1
\]  
(5.6)

is accurate to \( 10^{-4} \). In this case, as it is confirmed by numerical experiment (figure 5.3), three positive and three negative diffraction maxima additional to the main transmitted peak are possible. For the same width and \( \Delta n = 3 \cdot 10^{-5} \) we get \( \nu = 0.3543 \) and

\[
J_0^2 + 2(J_1^2 + J_2^2) \approx 1
\]  
(5.7)

we have five diffraction maxima, see figure 5.3. For the \( \Delta n = 10^{-5} \), \( \nu = 0.1181 \) and

\[
J_0^2 + 2J_1^2 \approx 1
\]  
(5.8)

figure 5.3 shows only two additional maxima symmetric to the main peak. That is the case in the weak interaction regime, \( \nu \to 0 \) [11]. The case of the weak interaction regime (where \( \Delta n = 10^{-5} \)) brings us to the next numerical experiment. In the next section we choose the experimental conditions that give rise to only one diffraction peak, complementary to the main transmitted light beam. This condition of light and sound interaction is known as Bragg diffraction. Only under certain conditions the diffracted light adds up constructively to create a detectable signal.
5.4. The Light Beam Perpendicular Incidents on the Sound Field

Figure 5.2: Distribution of $EE^*$ in the detector plane. The sound wave is characterized by $\Lambda = 5.7 \cdot 10^{-3} cm$, $Q = 0.7736$, $\Delta n = 0$ (left) and $\Delta n = 10^{-5}$ (right), the medium is by $g = 0.99$, $\mu_s = 5 cm^{-1}$, width of the sound field is $w = 0.1 cm$, the number of the launched rays is $10^9$. 
Figure 5.3: Effect of $\Delta n$ on the distribution of $EE^*$ in the detector plane. The sound wave is characterized by $\Lambda = 5.7 \cdot 10^{-3} cm$, $Q = 0.7736$, the medium is by $g = 0.99$, $\mu_s = 5 cm^{-1}$, $w = 0.1 cm$, (a)–$\Delta n = 10^{-4}$, (b)–$\Delta n = 3 \cdot 10^{-5}$, (c)–$\Delta n = 10^{-5}$, the number of the launched rays – $10^{10}$
5.5 The Light Beam Obliquely Incidents on the Sound Field

In the next numerical experiment the light beam crosses the sound field with the angle $\alpha$ and the thickness of the layer $[z_u, z_u + w]$ is increased, figure 5.1. When the conditions $Q > \pi/2$ and $\alpha = \alpha_B$ (Bragg angle) are satisfied, it is possible to detect only the $0th$ order of the transmitted light and one additional maximum, the $-1th$ (or $+1th$). It is known that the width and the magnitude of the sound field determines the regime of light diffraction [10],[11]. Therefore, numerical experiments are made with different widths and amplitudes of the sound wave. The effects of the optical properties $\mu_s, g$ of the medium on the light and sound interaction regime is also investigated. As for the previous numerical experiments optical scatterers are present only in the sound-field, inside the layer $[z_u; z_u + w]$, figure 5.1.

5.5.1 The Sound Field with the Different Thicknesses

Here we perform simulation when the light beam obliquely falls on the plane sound wave. The parameters are adjusted so that $Q > 1$, where $Q = 2\pi \lambda_0 w / n_0 \Lambda^2$. We expect from the continuous theory that one large secondary maximum appears if the angle of incidence corresponds to the Bragg-angle. This means that the incident angle $\alpha$, between the direction of the light beam and the sound wave satisfies the condition $\cos \alpha = \lambda / 2\Lambda$, where $\lambda_0 = n_0 \lambda$, figure 5.1, (left). The thickness $w$ of the sound-layer is increased and all other parameters in the numerical experiment are kept constant. We perform the numerical experiment by the following conditions:

1) Turbid medium: $g = 0.99$, $\mu_s = 5cm^{-1}$, absorption is neglected.

2) Sound field: $w = 0.2cm, 0.5cm$ and $1cm$, the distance to the sound field is $z_u = 1cm$, the distance to the detector-plane is $a = 10cm$, see figure 5.1.
Chapter 5. Numerical Experiment

Items (3) (4) (5) are identical to the corresponding items in section 5.4.

6) Amplitude of the refractive index: $$\Delta n = 10^{-5}$$.

7) The light beam crosses the sound field with angle $$\phi_B = \pi/900$$, it enters the medium at $$x = 250$$ cells, $$y = 250$$ cells, $$z = 0$$, figure 5.1.

For these parameters the numerical experiments are carried out several times with different thicknesses of the sound field. The distributions of $$EE^*$$ at the detector-plane, when the Bragg condition is fulfilled are shown in figure 5.4. When the sound field is sufficiently thin, $$w = 0.2$$, the two addition symmetric maxima appear at the right and left side of the main un-deflected light peak. The position of these maxima can be calculated with assumption that the light beam obliquely incidents on the thin phase grid and $$Q < 1$$. When the thickness of the sound field is $$w = 1cm$$ we see only the transmitted (0–order peak) and one additional maximum (−1–order peak), figure 5.4. The position of the −1–order peak is calculated from the theory when $$Q > 1$$ for the Bragg diffraction regime.

We are now interested what happens when the amount of scattering processes in the medium decreases. Figure 5.5 presents result from the simulation when the thickness of the sound field is $$w = 1cm$$, $$w = 2cm$$, and $$w = 3cm$$ and the scattering coefficient is $$\mu_s = 1cm^{-1}$$. If we compare the case for $$w = 1cm$$, $$\mu_s = 5cm^{-1}$$ of figure 5.4 with the case $$w = 1cm$$, $$\mu_s = 1cm^{-1}$$ of figure 5.5, we see that the additional +1–order peak with a scattering coefficient $$\mu_s = 1cm^{-1}$$ even with $$Q \approx 8$$ is clearly visible. When the thickness is increased $$Q \approx 16$$ and $$Q \approx 23$$ case $$w = 2cm$$, $$w = 3cm$$ and $$\mu_s = 1cm^{-1}$$, the +1–order peak disappears, figure 5.5. With $$w = 3cm$$ and when the incident angle satisfies Bragg condition only two peaks (0–order and −1–order peak) appear, this fact coincides with the theory (section 4) when $$Q > 1$$. A similar picture is obtained if the width of the sound field is not very large so $$Q \approx 8$$, $$w = 1cm$$ but the rays experience many scattering processes, $$\mu_s = 5cm^{-1}$$, figure 5.4. We can explain this effect as follows. With an increasing scattering coefficient the ray path length in the sound field increases as well, consequently the region of the sound light interaction
5.5. The Light Beam Obliquely Incidents on the Sound Field

extends. From the continuum theory that means the transition from the Raman–Nath diffraction to the Bragg regime.
Figure 5.4: Effect of the different $w$ on the distribution of $EE^*$ when $\mu_s = 5cm^{-1}$, $g = 0.99$, $w = 0.2cm$, 0.5cm, 1cm, and $0.8 < Q < 7.7$, $\Delta n = 10^{-5}$, the light beam falls at the sound field with angle $\phi_B = \pi/900$, Bragg angle, the number of the launched rays is $3 \cdot 10^6$. 
Figure 5.5: Effect of the different $w$ on the distribution of $EE^*$ when $\mu_s = 1cm^{-1}$, all other parameters are the same as on the figure 5.4, the number of the rays is $3 \cdot 10^9$. 
5.5.2 The Sound Field with Different Scattering Coefficients

Let us show the transformation from Raman–Nath regime to Bragg diffraction when \( Q \approx 8 \), \( w = 1cm \). We keep all parameters of the simulation constant and vary only the scattering coefficient of the turbid medium from \( \mu_s = 1cm^{-1} \) to \( \mu_s = 7cm^{-1} \). This causes an increase of the scattering processes for the rays during their movement inside the medium. The numerical experiment is performed with the following conditions:

1) Turbid medium: \( g = 0.99 \), \( \mu_s = 7cm^{-1}; 1cm^{-1} \), absorption is neglected.

2) Sound field width is \( w = 1cm \), distance to the sound field: \( z_u = 1cm \), and distance to the detector plane: \( a = 10cm \), the light beam enters the medium at the point \( x = 250 \) cells, \( y = 250 \) cells, see figure 5.1(right).

The items (3) (4) (5) are identical to the items in the section 5.4.

6) The amplitude of the refractive index modulation is \( \Delta n = 10^{-5} \), the light beam obliquely incidents on the sound field under Bragg angle \( \phi_B = \pi/900 \).

The effect of the scattering coefficient \( \mu_s \) on the intensity distribution in the reference plane is shown in figure 5.6. When the number of scattering processes per ray increases then its path length in the sound-field increases, too. Consequently the region of the sound-light interaction enlarges, and as expected we obtain only one peak of the diffracted light , figure 5.6 when \( \mu_s = 7cm^{-1} \). The relatively large number of random scattering processes causes a reduction of rays scattered in the narrow angle defined by the Bragg condition. In addition, the increasing number of scattering events reduces the degree of coherence and adds noise to the transmitted and scattered radiation. Results presented in figure 5.6 suggest that the definition of \( Q \) as given (4.19) does not sufficiently characterize the light-sound interaction process in modified Monte Carlo model. In case of continuous theory the width of the sound beam is identical to the interaction length. In Monte Carlo simulation the interaction length has to be replaced by the number of interaction processes, this is the product of width \( w \) and
mean free path length $\rho_s = 1/\mu_s$. Keeping this in the mind the scattering coefficient of the medium can be estimated from the amplitude of the two additioned maxima at the right and left side of the main un-deflected light peak. The simulation performed above leads us to the assumption that the ability to detect the $+1-\text{order}$ peak (the right peak in the figure 5.6, when $\mu_s = 1cm^{-1}$) depends on the amount of rays launched into the medium. The additional $+1-\text{order}$ peak is sufficiently visible when the number of rays is $3 \cdot 10^9$, figure 5.5 (when $\mu_s = 1cm^{-1}$ and $w = 1cm$), and is barely visible in the background noise when only $10^8$ rays are launched. When $\mu_s = 7cm^{-1}$ it is necessary to launch $10^{10}$ photons to detect the $-1-\text{order}$ peak. Therefore the simulations shown in figure 5.6 were made for different numbers of launched rays. The distribution of $EE^*$ presented in all figures 5.6 is normalized by their maxima.

5.5.3 The Influence of the Number of the Launched Rays

It is evident, that the use of more random numbers yields to more accurate results because the precision of MC results is directly proportional to the square root of the random number size. Consequently the Monte Carlo model works well for a large number of rays and the results calculated by the simulation become more precise.

In figure 5.6 the number of rays required to detect all predicted maxima is $3 \cdot 10^9$ when $\mu_s = 1cm^{-1}$ and $10^{10}$ when $\mu_s = 7cm^{-1}$. For the results shown in figure 5.3 a number $10^{10}$ is required to detect all maxima predicted by theory, when the ray number is $10^9$ not all maxima are visible. In this section we compare the results of the modified Monte Carlo method for the ray numbers $10^8$, $10^9$ and $3 \cdot 10^9$. The numerical experiments were performed for two cases, when $Q \approx 8$, $Q \approx 23$ with the following conditions:

1) Turbid medium: $g = 0.99$, $\mu_s = 1cm^{-1}$, the absorption is neglected,
2) Sound field thickness: $w = 1cm$, $w = 3cm$. 
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Figure 5.6: Effect of the different $\mu_s$ on the distribution of $EE^*$ when $w = 1cm$ then $Q = 7.7355$, $g = 0.99$, $\mu_s = 1cm^{-1}$ and $\mu_s = 7cm^{-1}$, the sound wave $- \Lambda = 5.7 \cdot 10^{-3}cm$, $\Delta n = 10^{-5}$, the angle of incidence is $\phi_B = \pi/900$. 
5.5. The Light Beam Obliquely Incidents on the Sound Field

Items (3)(4)(5)(6) are identical to the items in the section above.

Figure 5.7 shows the $EE^*$ distribution in the detector plane for $\mu_s = 1cm^{-1}$ when $Q \approx 8$. The additional $+1$ – order peak (right peak in the figure) is sufficiently visible when the number of simulated rays is $3 \cdot 10^9$ and is barely visible in the background noise when only $10^8$ rays are launched in the medium. The simulation becomes different for higher $Q$, figure 5.8. With $Q \approx 23$ we see that even with the highest ray number investigated $3 \cdot 10^9$ the second diffraction peak remains invisible, as predicted in the theory for $Q > 1$, and only the whole simulation curve becomes smoother.
Figure 5.7: Effect of the number of rays on the distribution of $EE^*$, $Q \approx 8$, $\mu_s = 1cm^{-1}, g = 0.99$, the sound wave $\Lambda = 5.7 \cdot 10^{-3}cm, \Delta n = 10^{-5}$, the angle of incidence $\phi_B = \pi/900$, the number of rays (a) $- 10^8$, (b) $- 10^9$, (c) $- 3 \cdot 10^9$. 
Figure 5.8: Distribution of $EE^*$ in the detector plane, $Q \approx 23$, All other parameters the same as on the figure 5.7, the number of rays is $10^9$ and $3 \cdot 10^9$
5.5.4 The Effect of the Anisotropy Factor

Finally, we investigated the effect of the anisotropy factor on the intensity distribution of the modulated light. Results are shown in figures 5.9-5.11. Again the angle of incidence was kept constant and equal to the Bragg angle, $\phi_B = \pi/900$ as in the preceding sections.

Figure 5.9 depicts the variation of amplitudes of two diffracted peaks on the different anisotropy factors. The simulation is carried out with a relatively small scattering coefficient $\mu_s = 1cm^{-1}$ and the sound field parameter is equal to $Q \approx 8$ and $\Lambda = 5.7 \cdot 10^{-3}cm$, $\Delta n = 10^{-5}$. When the mean value of the scattering angle is $\langle \cos \theta \rangle = 0.99$ the scattering takes place mostly in the forward direction, the path length of the transmitted rays inside the light–sound interaction region is the shortest. The interaction between the light and sound waves is small under these conditions. Therefore, within the framework of wave theory we would say we are in the Ramann–Nath regime and two symmetric diffraction peaks appear in the simulation, figure 5.9. With decreasing anisotropy factor, the interaction length between the sound wave and the light wave increases. We gradually approach to the interaction regime of Bragg–scattering. This transition is very well reproduced by the decrease of one diffraction peak with decreasing anisotropy factor as shown in figure 5.9.

Figure 5.10 shows results from a similar simulation as before, the only difference is that a larger number of rays was used and the anisotropy factor is decreased to $g = 0.86$.

To investigate the effect of increasing the scattering coefficient $\mu_s$ inside the sound field when $g = 0.96$ and $g = 0.86$, the number of used rays has to be increased to $9 \cdot 10^9$ to generate results with a sufficiently low noise level, figure 5.11. Similar to the simulations performed in the section 5.5.2 we see that when the number of scattering processes increases, the region of the sound-light interaction enlarges, and only one peak of the diffracted light is visible. Comparing the results from figure 5.9 and figure 5.10 with results from figure 5.11 one sees that an increase in the scattering coefficient
5.5. **The Light Beam Obliquely Incidents on the Sound Field**

inside the sound field reduces the amplitude of the diffraction peaks on the right side of the central peak compared to that on the left peak. Again, this can be explained by the increase in the interaction zone due to the increase in the width of the sound wave in this case.
Figure 5.9: Distribution of $EE^*$ with the different anisotropy factors $g = 0.99, 0.96, 0.9$, the sound wave - $\Lambda = 5.7 \cdot 10^{-3} cm$, $\Delta n = 10^{-5}$, the medium - $w = 1 cm$, $\mu_s = 1 cm^{-1}$, the angle of incidence - $\phi_B = \pi/900$, the number of rays is $3 \cdot 10^9$.
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Figure 5.10: Distribution of $EE^*$ with the different anisotropy factors $g = 0.99, 0.9, 0.86$, the sound wave $\Lambda = 5.7 \cdot 10^{-3}cm$, $\Delta n = 10^{-5}$, the medium $w = 1cm$, $\mu_s = 1cm^{-1}$, the angle of incidence $\phi_B = \pi/900$, the number of rays is $6 \cdot 10^9$. 
Figure 5.11: Distribution of $EE^*$ with the different anisotropy factors $g = 0.96$, and $g = 0.86$, $\mu_s = 3cm^{-1}$, the number of rays is $9 \cdot 10^9$, all other parameters are the same as in the figure 5.10.
5.6 Different Amplitudes of the Refractive Index

The modified Monte Carlo method presented here can be compared with continuum theory described in [10], [11]. The simplest test for the novel method is that the positions of the diffracted peaks depicted in figures 5.2–5.10 are calculated from the well known theoretical formulas (see section 4). From the theory [10], [11] we know that in the interaction regime the parameters \( Q = \frac{2\pi w \lambda_0}{\Lambda^2 n_0} \) and \( v = \frac{2\pi \Delta n w}{\lambda_0} \) characterize the problem. The effect of the different thickness of the sound field was shown in section 5.5.1. Here we investigate the effect of the refractive index amplitude \( \Delta n \) on the intensity distribution of the scattered light, when the light beam interacts obliquely and orthogonally with the sound field, figures 5.12–5.17. We choose \( Q < 1 \) for the orthogonal incidence (figure 5.12 and figure 5.13) and \( Q > 1 \) for the Bragg angle, figures 5.14–5.17. The numerical experiments are performed for different anisotropy factors and scattering coefficients. As in all previous numerical experiments only rays are investigated, which experience at least one scattering processes inside the sound field.

5.6.1 Orthogonal Incidence

The simulations were performed for the light beam perpendicular incident on the sound field and \( Q < 1 \), the amplitude of the modulated refractive index \( \Delta n \in [10^{-5}, 3 \cdot 10^{-4}] \). We determine the maximum of each diffracted peak for each \( \Delta n \) (see for example figure 5.3), as result we get a set of points one for each \( \Delta n \). To show all three experimental sets in one figure we divided each curve by its maximum value, then the \(+1 – order\) is set to 0.35, and the \(+2 – order\) to 0.25. The lines in figure 5.12 and figure 5.13 are the squares of the Bessel functions of the 0, 1, 2 order, (see section 4), the numerical results are presented by asterisks (transmitted, \(0 – order\) peak), circles \( (+1 – order\) peak or \(-1 – order\) peak) and triangles \( (+2 – order\) peak or \(-2 – order\) peak). The results depicted in figure 5.12 and figure 5.13...
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Figure 5.12: Effect of the different $\Delta n$, when $w = 0.1\text{cm}$, $Q = 0.7735$, $g = 0.99$, $\mu_s = 10\text{cm}^{-1}$, solid curves show the square of the theoretical Bessel functions zero first and second orders, the numerical results are presented by asterisks (transmitted, 0–order peak), circles (+1–order peak) and triangles (+2–order peak).

provide good agreement between continuous theory and the numerical experiments performed by the modified Monte Carlo method. Figure 5.12 shows results for the simulations with anisotropy factor $g = 0.99$, the thickness of the sound field is $w = 0.1\text{cm}$, $Q \approx 0.8$ and scattering coefficient is $\mu_s = 10\text{cm}^{-1}$. The 0–order peak reflects the behavior of the transmitted peak, it contains quasi ballistic rays, rays that experience only a few scattering events. The results from numerical simulations of the 0–order peak for $g = 0.99$ (asterisks on the fig.5.12) don’t coincide completely with the theoretical curve. The results for the first and second order peaks coincide well with results from continuum theory in the range $0.5 << w2\pi\Delta n/\lambda < 2$ and deviate increasingly with growing parameter $w2\pi\Delta n/\lambda$ from the results of the theory, (figure 5.12).

If the anisotropy factor is smaller $g = 0.9$, see figure 5.13, all other param-
5.6. Different Amplitudes of the Refractive Index

Figure 5.13: Effect of the different $\Delta n$, when $w = 0.1\text{cm}$, $Q = 0.7735$, $g = 0.9$, $\mu_s = 10\text{cm}^{-1}$, solid curves show the square of the theoretical Bessel functions zero first and second orders, the numerical results are presented by asterisks (transmitted, $0$-order peak), circles ($+1$-order peak) and triangles ($+2$-order peak).

Parameters are the same as in figure 5.12, the simulation results better coincide with the theoretical curves. A large anisotropy factor means that the most rays are scattered in the forward direction. At a smaller anisotropy factor the scattering covers a higher scattering angle range and the relative number of rays scattered into the direction of the additional diffracted peaks increases and consequently the amplitude of the $0$-order peak decreases. We expect that with the decrease of the anisotropy factor $g \to 0$, and with a large number of rays launched in the medium, the simulation results would coincide with the theoretical curves from the continuous theory. The numerical results, presented in figures 5.12, 5.13, show that the scattering of coherent light in a random medium with a refractive index modulated by a plane sound wave has a similar behavior like the scattering of the incident...
light on the plane sound wave (section 4). If we consider for example scattering in a clear medium we have to investigate light scattering on molecules where the anisotropy factor is zero. Light is scattered equally in all directions (for unpolarized light or for light scattered perpendicular to the polarization plane of the incident radiation). For this case we would have no principal problem to generate the diffraction peaks for $Q < 1$. However, the calculation time needed would be extremely high. In effect, it seems to be well justified to neglect

5.6.2 Oblique Incidence of the Light Beam on the Sound Field

Here we simulate the effect of $\Delta n$ on the intensity distribution of the transmitted light, the light beam interacts under the Bragg angle with the sound field. For $Q > 1$ (the Bragg diffraction regime), we investigate only the $+1$ order deflected peak. For each value of the $\Delta n$ in the range $0 < \pi \Delta n w / \lambda_0 < 6$ the maximum of the peak is calculated. As a result we have a set of discrete points, each point corresponds to one value of $\Delta n$. Then the array of the simulated points is normalized by its maximum. From the continuum theory (see section 4, formula 4.40) we obtained the smooth curve in the figures 5.14–5.16, the numerical results are presented by the discrete points.

First we show the effect of the factor $Q$ that is clearly visible in figure 5.5. The simulations were performed for the different widths of the sound field ($w = 1 cm$, $w = 2 cm$, $w = 3 cm$), all other parameters were kept constant. Figure 5.14 shows the result for the $Q \approx 8$ (asterisks), $Q \approx 16$ (circles) and $Q \approx 23$ (diamonds), scattering coefficient is $\mu_s = 1 cm^{-1}$, $g = 0.99$ and the smooth curve depicts the results from continuum theory, see formula (4.40). Figure 5.14 shows that when $Q >> 1$, $Q \approx 23$ (diamonds), the simulation shows excellent agreement with the theory in the region $0.2 < 2 \pi \Delta n w / \lambda_0 < 4$. For $Q \approx 16$ (width of the sound field is $w = 2 cm$) the simulation points are shifted to the left, figure 5.14(circles). When $w =
1cm and $Q \approx 8$ the simulation result has its maximum at $2\pi \Delta nw/\lambda_0 \approx 1.9$, the result from continuum theory has its maximum at $2\pi \Delta nw/\lambda_0 = 3.1416$. This effect is also visible in figure 5.5, we see two additional peaks $+1$ and $-1$ order for $w = 1cm$, this explains that simulation points (asterisks) on the figure 5.14 don’t coincide with the theoretical curve. It

![Graph](image)

Figure 5.14: Effect of the different $\Delta n$ when the angle of incidence - $\phi_B = \pi/900$, for the different thickness of the sound field, the numerical results are presented by asterisks when $Q \approx 8$, circles when $Q \approx 16m$, and diamonds when $Q \approx 23cm$, result from the continuum theory - solid line, the medium - $g = 0.99$, $\mu_s = 1cm^{-1}$.

is interesting to investigate the effect of the refractive index amplitude $\Delta n$ if $Q \approx 8$ for different optical properties of the turbid medium. When $w = 1cm$ the amplitude of peaks on the detector plane depends on the optical properties of the turbid medium, figures 5.6, 5.9. First we perform numerical experiment for two different scattering coefficients $\mu_s = 1cm^{-1}$, and $\mu_s = 5cm^{-1}$, figure 5.15. With increasing scattering processes, $\mu_s =$
5 cm$^{-1}$, inside the sound field, the experimental points (asterisks in figure 5.15) deviate less from the theoretical curve than for the $\mu_s = 1$ cm$^{-1}$ (circles in figure 5.15). With extension of the scattering coefficient inside the sound field, the light and sound interaction region increases. We expect with increasing number of the scattering events per ray, the agreement between numerical results and theoretical curves becomes even better. Figure 5.16

![Figure 5.15: Effect of the different $\Delta n$ when the angle of incidence - $\phi_B = pi/900$, for the different $\mu_s$ of the medium, the numerical results are presented by the circles when $\mu_s = 1$ cm$^{-1}$, and asterisks when $\mu_s = 5$ cm$^{-1}$, result from the continuum theory - solid line, the medium - $g = 0.99$, $w = 1$ cm.](image)

shows the effect of the $\Delta n$ on the intensity distribution of the transmitted light for two value of the anisotropy factor $g = 0.99$ and $g = 0.9$, when $Q \approx 8$. The deviation of the simulation points from the theoretical curve does not change much if the anisotropy factor is varied. The anisotropy factor of the medium has not much influence on the numerical results depicted in figure 5.16. The results presented in the figures 5.12–5.16 show that with
Figure 5.16: Effect of the different $\Delta n$ when the angle of incidence - $\phi_B = \pi/900$, for the different anisotropy factors of the medium, the numerical results are presented by the circles when $g = 0.99$, and diamonds when $g = 0.9$, result from the continuum theory - solid line, the medium - $w = 1cm, \mu_s = 1cm^{-1}$.

our modified Monte Carlo Method (based only on the scattering processes inside the sound field), the light diffraction on the plane sound wave can be successfully simulated. The results from the numerical simulations show good qualitative agreement with the theoretical curves, figure 5.13, when the light beam incidents orthogonally on the sound field as well as if the light beam incidents under Bragg angle, figure 5.14. It is not much surprising that for Monte Carlo simulation of the interaction of a plane wave with a sound wave scattering processes outside of the sound field are unimportant and can actually be neglected. The same is done in continuum theory. Considering the difference between the Monte Carlo simulation and the continuum theory there are two main differences: In our simulation we consider a light beam with finite width, we do not
simulate a plane wave. For practical research we have a relatively high anisotropy factor in contrast to molecular scattering.

5.7 Scattering in front of the Sound Field

In previous sections the light beam propagates in the medium where the optical scatterers exist only in the sound field. Up to this point the modified Monte Carlo method was used and the effect of a sound wave that modulates the index of refraction of the medium was investigated. The method showed that when a light beam incidents on the sound field at the Bragg angle only one diffracted peak can be detected. For the formation of this peak only the scattered light participates. Now we add scattering processes in the region in front of the sound beam, and the angle of incidence of a light beam to the sound field is the Bragg angle, \( \phi_B = \pi / 900 \), figure 5.1(left). Scattering outside of the sound wave would mainly add noise. Qualitatively, we do not expect much influence on the scattering processes outside of the sound wave. Additional scattering outside the sound wave demands an increase of number of rays in the medium and as a consequence the computational time increases. The first step is to add scattering processes only in front of the sound field, in section 5.9 we add scattering behind the sound field. All previous simulations (figures 5.2–5.16) were performed with the assumption that all rays have been incident under the same angle on the sound field, now this angle is varied statistically due to scattering processes in front of the sound wave. We perform numerical experiments as it is shown in figure 5.1(left), but the region before the sound field is a turbid medium (\( g < 1 \)).
5.7. Scattering in front of the Sound Field

Figure 5.17: Distribution of $EE^*$ in the detector plane, the light beam crosses the sound field under angle $\phi_B = \pi/900$, the sound wave – $\Lambda = 5.7 \cdot 10^{-3} \text{cm}$, $\Delta n = 10^{-5}$, the medium – $w = 2 \text{cm}$, $\mu_s = 1 \text{cm}^{-1}$, $g = 0.99$, the turbid medium occupies the region $[0; z_u + w]$, $z_u = 1 \text{cm}$–left, and $z_u = 3 \text{cm}$–right.
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The simulations, with results shown in figure 5.17, were carried out with\( g = 0.99\) inside the sound field, and in front of the sound layer, so the whole region which is occupied by the turbid medium is \([0; z_u + w]\), (see figure 5.1, left). After passing this region the scattered rays propagate straightforward. The parameters were taken for the case when only one first order peak is visible (Bragg interaction regime and \( Q > 1 \)) and the width of the sound field is \( w = 2cm \). Figure 5.17 shows result from two simulations, one has been made for \( z_u = 1cm \) and another when \( z_u = 3cm \), where \( z_u \) is the thickness of the turbid medium in front of the sound wave. The first order diffracted peak is barely visible when thickness \( z_u \) of the turbid medium in front of the sound field increases. The scattering outside the sound beam region effectively leads to a reduction of rays that constructively interfere and consequently the Bragg peak is reduced.

![Figure 5.18: Effect of the refractive index amplitude \( \Delta n \). Medium – \( w = 2cm, \mu_s = 1cm^{-1}, Q > 1, \ g = 0.99 \), circles – simulation without scattering in front of the sound field, diamonds – scattering before the sound field \( z_u = 1cm \), asterisks – scattering before the sound field \( z_u = 3cm \). The solid line is the theoretical result.](image-url)
5.7. Scattering in front of the Sound Field

Figure 5.18 shows the effect of the refractive index amplitude $\Delta n$ on the intensity of the transmitted sound-modulated light for oblique incidence of the diffused light beam on the sound. We analyze here results depicted in figure 5.17 for the two cases $z_u = 1cm$ and $z_u = 3cm$. The refractive index amplitude $\Delta n$ is varied in the range $0 < 2\pi\Delta n w/\lambda_0 < 6$. We determine the maxima for each $\Delta n$. From the continuum theory we obtained the solid line, the numerical results are presented by the discrete points. The set of points depicted as circles shows simulation results when scattering is included only inside the sound field (the same results presented by circles in the figure 5.14), the diamonds represent results for the simulation when optical scatterers exist in front of the sound for $z_u = 1cm$. The asterisks are results when $z_u = 3cm$, the turbid medium occupies the region $[0; z_u + w]$. The simulation points (circles) for the case without optical scatterers outside the sound field almost coincide with points represented result with the scattering before the sound (diamonds), when $z_u = 1cm$. The simulation curve of points (asterisks, for $z_u = 3cm$) is broader then the curve of the diamonds presented case for $z_u = 1cm$. We can assume that with increasing of the number of launched rays in simulation the points depicted the results for the scattering before the sound when $z_u = 3cm$ approach to the points depicted as diamonds ($z_u = 1cm$), see figure 5.18. We see that there is no sufficient influence of scattering processes outside of the sound wave on the simulation results for the different refractive index.

Figure 5.19 shows results for the next numerical experiment performed when scattering is present in front of the sound field for $z_u = 5cm$. All other simulation parameters are the same as in figure 5.17. The optical properties of the turbid medium are $\mu_s = 1 cm^{-1}$, $g = 0.99$. The light beam falls with Bragg angle on the sound field with a width of $w = 1cm$. When $Q \approx 8$ and the scattering is included in front of the sound field thickness $z_u = 5cm$, only one peak is visible, in contrast to the results of the simulation without scattering (see, figure 5.5), for $w = 1cm$. With the scattering in front of the sound field and $\Delta n = 10^{-5}$, figure 5.19(a), only one transmitted peak is visible. If the amplitude of the variation of the index of refraction by the sound field is increased to $\Delta n = 2.5 \cdot 10^{-5}$ then $-1$–order peak and $0$–order
peak (transmitted) are visible (figure 5.20(b)), and with $\Delta n = 4 \cdot 10^{-5}$ we see only one deflected $-1$–order peak, figure 5.19(c).
5.7. Scattering in front of the Sound Field

Figure 5.19: Distribution of $EE^*$ on the detector plane, for different $\Delta n$,
(a) $\Delta n = 10^{-5}$, (b) $\Delta n = 2.5 \cdot 10^{-5}$, (c) $\Delta n = 4 \cdot 10^{-5}$, medium–
$z_u = 5\text{cm}$, $w = 1\text{cm}$, $\mu_s = 1\text{cm}^{-1}$, $Q > 1$, $g = 0.99$, the ray
number is $5 \cdot 10^{10}$.
The effect of the amplitude $\Delta n$ of the refractive index when optical scatterers are present in front of the sound beam and $z_u = 5cm$ is presented in figure 5.20. The refractive index amplitude is varied in the range $0 < 2\pi\Delta nw/\lambda_0 < 6$. The circles are simulation results for the scattering only inside the sound field and $w = 1cm$, as already shown in the figure 5.14. The simulation results (diamonds in figure 5.20) for scattering in front of the sound field with $z_u = 5cm$ do almost coincide with results (circles) when optical scatterers exist only in the sound field. We should point out that the amount of the rays required for the simulation with scattering in front of the sound field with $z_u = 5cm$ is $5 \cdot 10^{10}$, and simulation time was more than two weeks.

Figure 5.20: Effect of the refractive index amplitude $\Delta n$, medium -- $w = 1cm$, $\mu_s = 1cm^{-1}$, $Q > 1$, $g = 0.99$, for circles -- scattering only inside the sound, diamonds -- scattering in front of the sound beam and $z_u = 5cm$. The solid line represents the theoretical result.

The previous simulations with the scattering in front of the sound field were performed for the scattering coefficient $\mu_s = 1cm^{-1}$. The following
5.7. Scattering in front of the Sound Field

Simulations were calculated with $\mu_s = 5 \text{cm}^{-1}$. The other simulation parameters are: width of the sound beam is $w = 1 \text{cm}$, and $z_u = 1 \text{cm}$, anisotropy factor is $g = 0.99$. The effect of $\Delta n$ is presented in figure 5.21. For comparison we show the simulation results (circles) with scattering only inside the sound field for $\mu_s = 5 \text{cm}^{-1}$ (the same points as in figure 5.15). Then we add scattering processes in the region $[0; z_u]$, the numerical results for the different amplitude of the refractive index are depicted by the diamonds in figure 5.21. We see that two arrays of the simulation points almost coincide.

The next step in the simulation was the expansion the sound beam width to $w = 3 \text{cm}$, in this case $Q >> 1$ and we are well within the Bragg diffraction regime. The optical scatterers are in front of and inside the sound beam. The other parameters are: $z_u = 1 \text{cm}$, $\mu_s = 1 \text{cm}^{-1}$, the angle of incidence is the Bragg angle. Simulations were made for two different anisotropy factors $g = 0.99$ and $g = 0.96$. Figure 5.22 shows the effect of $\Delta n$ on the intensity distribution of the modulated light. We see that in the range $0.0 < 2\pi\Delta n w/\lambda_0 < 6$ the simulations points well coincide with the theoretical results and there is no big difference between results for $g = 0.99$ (asterisks in figure 5.22) and results for $g = 0.96$ (circles in figure 5.22). The solid curve represents the theoretical results, from formula (4.40). It is interesting that in the region $6 < 2\pi\Delta n w/\lambda_0 < 12$ the second maximum in the simulation "curves" is well visible. The amplitudes of these two maxima are different for the two values of the anisotropy factor. For the larger range of the scattering angle $g = 0.96$ the second maximum of the simulation results approaches the theoretical results and it is larger than the second maximum for $g = 0.99$. We should point out that this effect is only obtained if scattering is present in front of the sound beam. It is essential to mention that for all simulations done before in the case when the sound field width is $w = 1 \text{cm}$ and $w = 2 \text{cm}$, and when light beam falls on the sound field at Bragg angle, figures 5.14-5.16, figures 5.18,5.19 the range $6 < 2\pi\Delta n w/\lambda_0 < 12$ was also simulated but the simulation results show no maximum in this range. As a conclusion the effect of scattering in the region in front of the sound beam on the intensity distribution of the transmitted light was
investigated. The simulations were carried out for various widths of the sound field \( w = 1cm, w = 2cm, w = 3cm \) and different optical properties of the turbid medium. The distance between the source plane and the sound beam was also varied. We see that there is no significant influence of the scattering processes outside of the sound wave on the simulation results when the width of the sound is \( w = 1cm \) and \( w = 2cm \) \((Q > 1)\). We expect that with increasing ray numbers the results for the scattering before the sound field approach the results without scattering. The influence of the scattering in front of the sound beam is visible only for the case when \( Q >> 1 \), \( w = 3cm \), figure 5.22. We see a second maximum when \( \Delta n \) is in the range \( 6 < 2\pi\Delta nw/\lambda_0 < 12 \). When scattering outside the sound field is included in the simulation the number of the launched rays are necessary to increase and as a consequence the computational time increases, too.

Figure 5.21: Effect of the refractive index amplitude \( \Delta n \) for \( \mu_s = 5cm^{-1} \), medium – \( w = 1cm, Q > 1, g = 0.99 \), diamonds – simulation with scattering in front of the sound field, circles — scattering only inside sound field.
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Figure 5.22: Distribution of $EE^*$, medium – $z_u = 1\, cm$, $w = 3\, cm$, $\mu_s = 1\, cm^{-1}$, $Q > 1$, simulation with scattering in front of the sound field, $g = 0.99$–asterisks, $g = 0.96$–circles. The smooth curve represents the theoretical results.
Chapter 5. Numerical Experiment

5.8 Doppler Effect in the Modified Monte Carlo Method

The main purpose of this project is to develop a method that can detect among diffused transmitted light the light tagged by the ultrasound wave. This effect permits scattered light that has traversed a specific localized region to be distinguished from all other diffused light. The concept under investigation in this section is to add frequency marks to the rays by interaction with the sound wave.

In the model of the light propagation in the turbid medium presented here the light scattering occurs on the inhomogeneities of the medium. These inhomogeneities can be described as the spatial variations of the refractive index of the medium. In the Monte Carlo model of light propagation in the turbid medium the variations of the refractive index are represented by the scattering centers. In our model we assume that when the light beam crosses the sound field the scattering centers now represent the periodic variation of the refractive index in space, see formula (5.1), and therefore we can assume that the scatterers in the sound wave move with a speed of sound as well.

Because the sound travels through the medium with a finite velocity, rather than remaining stationary in space, the acoustic wave Doppler-shifts the frequency of the diffracted light beam [10]. The phase grid generated by the sound wave moves through the medium with the speed of sound. Since optical frequencies are much greater than acoustic frequencies, the variations of the refractive index in a medium are very slow in comparison with optical period. In correspondence to our model this fact is described as follows, the lifetime of a ray in the turbid medium is much shorter than the time of the displacement of the scatterers due to the sound field. To take the frequency shift into account we assume that each scatterer in the sound field has the velocity \( v_s \). The frequency of the ray propagated in the
5.8. Doppler Effect in the Modified Monte Carlo Method

sound field after the $j$–scattering event is that

$$\omega_j = \omega_{j-1}(1 + \frac{v_s}{c} \sin \theta_{j-1}),$$

(5.9)

where $\theta_j$ is the scattering angle calculated by Monte Carlo method and corresponds to the $j$ scattering event, $\omega_{j-1}$ is the shifted frequency from the interaction with the preceding scatterer. When the frequency-shifts are included in our simulation, this leads to the same intensity distribution of the transmitted modulated light as it is presented in figure 5.5 or figure 5.6. If a ray passed through the sound field his frequency is shifted and calculated by formula(5.9). We induce a frequency filter in our simulation, its function is to detect rays with frequencies shifted by the sound wave. The filter is located on the detector plane, and the intensity distribution of the transmitted modulated light is calculated for the light "tagged" by the sound wave. Figure 5.23 presents the intensity distribution of the sound modulated light in the detector plane. The light beam obliquely incidents on the sound field under Bragg angle $\phi_B = \pi/900$. The results on the left are from the simulation with frequency filter and on the right are without the filter. Only one maximum is visible, as it is shown in figure 5.23(left) with the frequency filter. The frequency filter used for this simulation selects photons whose frequency shifts are in the range $-\Omega \cdot 1.1 < \Delta \omega < -\Omega \cdot 0.9$. 

![Figure 5.23: Distribution of $EE^*$ on the detector plane using a frequency filter (left) and without filter (right), turbid medium - $w = 3cm$, $g = 0.99$, $\mu_s = 1cm^{-1}$, the sound wave - $\Lambda = 5.7 \cdot 10^{-3}cm$, $\Delta n = 10^{-5}$, the angle of incidence is $\phi_B = \pi/900$.](image)
Figure 5.24: Distribution of $EE^*$ on the detector plane, $\Delta n = 10^{-5}$, medium--$w = 2cm, \mu_s = 1cm^{-1}$, $g = 0.99$. Distribution of $EE^*$ in the detector plane with the different frequency filters, turbid medium - $w = 3cm$, $g = 0.99$, $\mu_s = 1cm^{-1}$, the sound wave - $\Lambda = 5.7 \cdot 10^{-3} cm$, $\Delta n = 10^{-5}$, the angle of incidence is $\phi_B = \pi/900$.

If the filter is removed (figure 5.23, right) the zero–order undiffracted peak (right spot) appears.

Figure 5.24 shows the cross section of the intensity distribution of the modulated light presented in figure 5.23. The two maxima at the position $y = 230 cells$ in figure 5.24 represent the results from two frequency filters. The maximum obtained with the frequency filter $-\Omega \cdot 1.2 < \Delta \omega < -\Omega \cdot 0.8$ well coincides with the result without filter. The other maximum represents results for the frequency filter in the range $-\Omega \cdot 1.1 < \Delta \omega < -\Omega \cdot 0.9$. For the simulations presented below the frequency filter in the range $-\Omega \cdot 1.2 < \Delta \omega < -\Omega \cdot 0.8$ was used.

The effect of the refractive index amplitude $\Delta n$ on the intensity distribution of the transmitted light when a frequency filter is applied, is shown in
5.8. Doppler Effect in the Modified Monte Carlo Method

Figure 5.25. For the results in the figure 5.25 only the peak obtained with frequency filter (see figure 5.23) was investigated. We compare the simulation results obtained with the frequency filter with the results depicted in figures 5.14–5.16. For each value of $\Delta n$ in the range $0 < 2\pi\Delta nw/\lambda_0 < 6$ the intensity distribution of the transmitted light with the frequency filter was simulated. From continuum theory we obtained the smooth curve shown in figure 5.25. The numerical results are presented by the sets of discrete points (circles and diamonds). The light beam incidents on the sound beam under Bragg angle $\phi_B = \pi/900$, the simulations were performed for $w = 1$cm (figure 5.25, left) and $w = 2$cm (figure 5.25, right). The points depicted as circles correspond to the numerical results obtained without frequency filter (see for example figure 5.14 asterisks for $w = 1$cm and circles for $w = 2$cm). Figure 5.25 shows that the peak simulated with the frequency filter have the same behavior as the Bragg peaks obtained only due to constructive interference of the diffused photons (figure 5.14). We should point out that for obtaining stable results with a frequency filter we launched less rays than for the simulation without filter.

Figure 5.25: Effect of the different $\Delta n$ for different thicknesses of the sound field, results with the frequency filter are presented by diamonds and without the filter by circles, result from the continuum theory - solid line, the medium - $g = 0.99$, $\mu_s = 1$cm$^{-1}$, $\phi_B = \pi/900$. 

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5.9 Scattering in front of and behind the Sound Beam

The effect of the scattering in front of the sound wave on the intensity distribution of the transmitted light was investigated in section 5.7. Qualitatively, there is not much influence of scattering processes outside of the sound wave. Now the scattering in front of and behind the sound field is included in the simulation. The results in figures 5.17, 5.19 show that with scattering in the region before the sound field the amount of rays that constructively interfere decrease and the Bragg peaks reduce. Now we are approaching the main question of our project: Is it possible to detect the light tagged by the sound wave among all transmitted light? In this section we add scattering to the region behind, and in front of the sound beam. To detect the light "tagged" by the sound beam, the frequency filter is used.

The geometry of our simulation is as follows: The turbid medium ($g < 1$) occupies the region $[0; z_u]$ in front of the sound beam and the region $[z_u + w; (z_u + w) + w_1]$ behind the sound beam and $w_1 < a$ (see figure 5.1). This region is not displayed in figure 5.1. After passing the region $[0; (z_u + w) + w_1]$ the scattered rays propagate in straight direction. The angle of incidence of the light beam on the sound field remains the Bragg angle, $\phi_B = \pi/900$. The frequency filter is introduced in the detector plane and selects the light "tagged" by the sound beam. For the results presented in this section, a frequency filter $-\Omega \cdot 1.2 < \Delta \omega < -\Omega \cdot 0.8$ is chosen.

The intensity distribution of the transmitted modulated light when scattering takes place the region $[0; (z_u + w) + w_1]$ is presented in figure 5.26. The effect of scattering outside the sound field becomes visible when we compare results in figure 5.26, left with the results in the figure 5.26, right. The simulation was carried out for a sound beam width of $w = 3cm$. All parameters are the same as for the figure 5.5, when width $w = 3cm$. Figure 5.26 shows the cross section of the intensity distribution with and without frequency filter. The results without scattering outside the sound
are presented in figure 5.26,left. When the turbid medium occupies region \([0;(z_u+w) + w1]\), the intensity distribution of the transmitted light is shown in figure 5.26,right. Light scattering in the region outside the sound field reduces the peak amplitude of the diffracted beam, as expected. However, the use of the frequency filter allows to detect among all diffused transmitted light, the light "tagged" by the sound wave.

Figure 5.26: Distribution of \(EE^*\) in the detector plane, medium - \(w = 3cm, z_u = 1cm, \mu_s = 1cm^{-1}, g = 0.99, w_1 = 1cm\), the sound wave - \(\Lambda = 5.7 \cdot 10^{-3}cm, \Delta n = 10^{-5}, \phi_B = \pi/900\), results without scattering outside the sound field are presented in the left figure, and with the scattering – in the right figure.

We see that the Bragg peak almost vanishes when the scattering in front of and behind the sound field is included (figure 5.26 right), but with the frequency filter it is still visible. Next we investigate the evolution of the peak obtained with the frequency filter for the scattering in front of and behind the sound wave when the amplitude of the refractive index is in the range \(0 < 2\pi \Delta n w / \lambda_0 < 6\). The first simulation is performed for a small scattering coefficient \(\mu_s = 1cm^{-1}\) and width of the sound field \(w = 1cm\). Without the scattering in front of and behind the sound field we obtain
with frequency filter the set of points depicted as diamonds in figure 5.27. The circles represent result without the frequency filter, when scattering is only inside the sound beam, figure 5.27. The asterisks show results obtained with frequency filter and when the scattering in front of and behind the sound wave is included for $w_1 = 1\text{cm}$. We see from the results presented in figure 5.27 that the scattering in front of and behind the sound field has no influence on the behavior of the results. With increasing the numbers of propagated rays the simulation results with scattering will better coincide with results without scattering.

The evolution of the peak obtained with the frequency filter (see figure 5.26) for the scattering outside the sound field when $\Delta n$ is in the range $0 < 2\pi \Delta n w / \lambda_0 < 6$ and $w = 3\text{cm}$ is presented in figure 5.28. For comparison we present results from three independent simulations. The circles represent results without frequency filter with scattering only inside the sound (the circles in figure 5.28 or diamonds in figure 5.14). The diamonds on the figure 5.28 depict results with frequency filter, when scattering only is inside the sound. And the asterisks in the figure 5.28 show results from the simulation with frequency filter when scattering is in front of and behind the sound field and $w_1 = 1\text{cm}$. We see that the curve indicating by the asterisks is broader than the curve with diamonds. This can be explained as, when the scattering is included in the simulation this yields to decreasing number of rays reaching the detector plane. When the scattering is included in the simulation this yields to an expansion of the ray number used in the experiment and as a consequence the computational time increases, too.
5.9. Scattering in front of and behind the Sound Beam

Figure 5.27: Effect of the refractive index amplitude $\Delta n$, medium – $w = 1\text{cm}$, $z_w = 1\text{cm}$, $\mu_s = 1\text{cm}^{-1}$, $g = 0.99$, the sound wave - $\Lambda = 5.7 \cdot 10^{-3}\text{cm}$, $\phi_B = \pi/900$. the circles - results without the frequency filter, when the scattering only is inside the sound beam, the diamonds - results with the frequency filter, when the scattering only is inside the sound beam. the asterisks - results with the frequency filter, when the scattering is in front of and behind the sound beam, smooth curve represents the theoretical result.
Figure 5.28: Effect of the refractive index amplitude $\Delta n$, medium $w = 3cm$, $z_u = 1cm$, $\mu_s = 1cm^{-1}$, $g = 0.99$, the sound wave $\Lambda = 5.7 \cdot 10^{-3}cm$, $\phi_B = \pi/900$. The circles - results without the frequency filter, when the scattering is only inside the sound beam, the diamonds - results with the frequency filter, when the scattering only is inside the sound beam. The asterisks - results with the frequency filter, when the scattering is in front of and behind the sound beam, smooth curve represents the theoretical result.
Chapter 6

Summary and Conclusion

We have calculated the local intensity distribution of light after passage through a scattering region whose index of refraction is modulated by a sound wave. The phase of the rays is calculated by tracing their optical path length. The sound wave is represented by a periodic phase modulation of the medium. We could successfully simulate the occurrence of scattering maxima if the Bragg condition is fulfilled. The appearance of higher order "diffraction peaks" and even the validity of the Bragg condition were shown in the simulation, when only scattering processes in the layer with the sound field were considered. In most case only rays were investigated, which experience at least one scattering processes in the sound field. We obtained by modified Monte Carlo method that the magnitude of the Bragg peak, which appears only due to the constructive interference of the phase modulated light, is governed by the thickness of the sound field, the scattering coefficient, the anisotropy coefficient of the medium and the number of launched photons. The results presented in the section 5.6 show that our modified Monte Carlo Method based only on scattering processes can successfully simulate the light diffraction on a plane sound wave. The results from the numerical experiment show good agreement with theoretical curves, when the light beam incidents orthogonal on the sound field and when the light incidents with Bragg angle, section 5.6. The
simulation reveals that the light scattered only on the optical scatterers in the region with the sound field shows behavior similar to light scattering on the plane sound wave in transparent homogeneous medium.

First we neglected scattering processes outside of the sound wave. Scattering outside of the sound wave would add noise. Qualitatively, we do not expect much influence of scattering processes outside of the sound wave. The main purpose of this project is to develop method that can detect among diffused transmitted light the light tagged by the ultrasound wave. This effect permits that a scattered light that has traversed a specific localized region can be distinguished from all other scattered light. In section 5.8 we extended to model to the treatment of frequency shift included by the Doppler effect. We introduced a frequency filter in our simulation. Its function is to detect rays with frequencies shifted by the sound wave. In the model presented here this filter is located in the detector plane, and the intensity distribution of the transmitted modulated light is calculated only for the light "tagged" by the sound wave. Results presented in section 5.8 show that the peak simulated with the frequency filter have the same behavior as the Bragg peak obtained only due constructive interference of the scattered light.

The next step was to add scattering processes before and after the sound, section 5.9. The simulations were carried out for the various width of the sound field and different optical properties of the turbid medium. The distance between the source plane and the sound beam is also varied. We expect that with increasing the photon number the simulation results for the scattering outside the sound approach to the results obtained without scattering. We should point out that when scattering is included in the simulation the number of the launched photons in medium sufficient increases and as consequence the computational time increases too.

In our project the modified Monte Carlo modeling of the light propagation in a turbid medium with the layer contains the sound plane wave was developed. It was shown that among diffused transmitted light can be detected the light tagged by the ultrasound wave. This effect gives oppor-
tunity to distinguish from all scattered light, the light that has traversed a specific localized region.
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