Numerical simulation of
diffraction of a Gaussian beam
near an atom chip

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Abstract

Optical beams can be used in experiments with ultra-cold gases to confine and manipulate atoms. Examples include dipole traps, optical lattices and Bragg/Raman scattering. These methods provide an entry to studying fundamental phenomena, such as interactions in many-body quantum systems. In the CELSIUS setup, a cold gas is created using laser-cooling and confined in a magnetic field 50-100 µm below an atom chip. Due to the small spatial separation between the gas and the chip, optical beams focused on the gas will diffract, both from the edge of the chip and from obstacles on it. This distortion of the beam can perturb the intensity pattern in the region of the gas and possibly affect any experiments. Numerical methods are employed to study the effect of diffraction from the edge and reflection from the chip surface, using both scalar diffraction theory and finite-difference time domain analysis. Feasability of FDTD analysis for more complex chip geometries is examined.
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1. Introduction

Background: CELSIUS setup & optical potentials

This thesis revolves around optical beams that are used to manipulate cold atoms in the CELSIUS[1, 2] setup (Chip Experiment for Low-dimensional Strongly Interacting Systems). The CELSIUS setup is a system for creating and maintaining an ultra-cold gas and consists of an ultra-high vacuum system, in which $^{87}\text{Rb}$ atoms are injected by resistive heating of a dispenser in the chamber. Counter-propagating laser beams, locked close to a resonant transition of $^{87}\text{Rb}$, are then used to cool the atoms after which they are confined in a magnetic trap that is produced by an atom chip and external coils. Once trapped, evaporative cooling is employed to obtain a one dimensional ultra-cold gas and optical beams can then be used in a variety of ways to manipulate or confine these cold-atoms. This provides a way of studying fundamental phenomena, such as interactions in many-body quantum systems, in a very controlled matter and may also provide a means for constructing quantum registers for use in quantum computation. Optical beams can manipulate atoms because the electric fields of the beam, when the beam is detuned from any resonant transitions, can induce an electric dipole moment in the atoms. This dipole moment then interacts with the electric field of the laser and the atom experiences a dipole force. Depending on whether the beam is detuned below or above the resonant frequency of the atom, this force will either be pulling it towards or away from the intensity maxima.

By controlling the geometry of the optical potential, the beam detuning and the intensity, very precise control over the cloud can be obtained. One can use this to produce dipole traps, where a single beam provides a strong trapping potential, optical lattices, by interfering multiple counterpropagating beams, or perform Bragg/Raman scattering, by using counter-propagating pulses of slightly detuned beams.

In the experimental setup that is being used at the Van der Waals-Zeeman Institute, an optical beam with a wavelength near 780 nm, is focused on a 1D cold gas of $^{87}\text{Rb}$ atoms confined by a magnetic field 50 – 100 $\mu$m below an atom chip. Due to the small spatial separation of the cold gas and the atom chip it is inevitable that the beam will diffract from obstacles on and from the edge of the chip. This distortion of the beam can perturb the intensity pattern in the region of the gas and affect the experiment. In this thesis, numerical models are used to study the effects of diffraction on the optical potential, and these are used to calculate the field under the chip for simple geometries.

Geometry of setup

The cold atom experiments at the Van der Waals-Zeeman Institute are performed with an atom chip, positioned in an ultra-high vacuum chamber to prevent collisions with the background gas. The atom chip itself is a patterned microconductor consisting of gold wires. These wires generate, in combination with external coils, a magnetic trapping potential used to produce a confinement for an ultra-cold gas. An image of the atom chip is shown in figure (1): it measures 25 x 16 mm and consists of a silicon monocrystal substrate on which gold wires are deposited. Gold was chosen both for its high reflectivity at $\lambda = 780$ nm ($\approx 98\%$) and high conductivity (required for the high currents to generate the magnetic fields). On the surface of the chip are undercuts, several micron deep, to separate the gold wires.
varying the current through the wires, the minimum of magnetic potential and thus the position of
the cold gas can be controlled in the region between 25-100 µm. As shown in figure 2 a substantial part
of the beam, when focused on the atomic cloud, impinges on the edge of the chip.

Figure 2: Diffraction geometry: the atom chip, suspended upside-down, confining a cold-gas 50-100
µm below the surface, with the laser impinging on it from the left.

Overview of the report

The outline of the thesis will follow the following structure:

- **Section 2**: Theoretical background with a mathematical treatment of laser beams and scalar
diffraction theory
- **Section 3**: Effects of diffraction on power loss, diffraction of a Gaussian beam by a half plane
and discussion of the numerical implementation. Several techniques for calculating diffraction
are then used to calculate patterns relevant for the optical experiment
- **Section 4**: A consideration and model to include reflection from the chip surface in the intensity
patterns.
- **Section 5**: Basic theory of time-domain simulation and feasibility study for doing FDTD analysis
on the atom chip.
- **Section 6**: Conclusion and outlook
2. Theoretical background

2.1 Electromagnetic fields & Maxwell’s equations

Maxwell’s equations are a set of partial differential equations that describe how electric and magnetic fields are generated by charges and currents and how these fields influence each other. Maxwell’s equations in matter, that are derived from Maxwell’s fundamental equations by including the polarization \( P \) and magnetization \( M \) of the material are

\[
\begin{align*}
\nabla \cdot \mathbf{D} &= \sigma_f \quad \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \cdot \mathbf{B} &= 0 \quad \nabla \times \mathbf{H} = \mathbf{J}_f + \frac{\partial \mathbf{D}}{\partial t}
\end{align*}
\]

Here \( \mathbf{D} \) is the displacement field \( \mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P} \) and \( \mathbf{H} = \mathbf{B}/\mu - \mathbf{M} \) the magnetic H-field. The free charge and current density are denoted \( \sigma_f \) and \( \mathbf{J}_f \). In the absence of free charges we have \( \sigma_f = 0 \), from which follows that \( \mathbf{J}_f = 0 \), these equations then reduce to

\[
\begin{align*}
\nabla \cdot \mathbf{D} &= 0 \quad \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \cdot \mathbf{B} &= 0 \quad \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t}
\end{align*}
\]

If we only consider homogeneous, linear, isotropic dielectric we can then approximate \( \mathbf{D} = \varepsilon \mathbf{E} \), \( \mathbf{H} = \mathbf{B}/\mu \), where \( \varepsilon \) and \( \mu \) are constants: if the medium were non-homogeneous \( \varepsilon \) would be a function of position, if it were anisotropic, it would be a tensor. Using these approximations we obtain

\[
\begin{align*}
\nabla \cdot \varepsilon \mathbf{E} &= 0 \quad \nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t} \\
\nabla \cdot \mathbf{B} &= 0 \quad \nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t}
\end{align*}
\]

This is a set of coupled first order partial differential equations. They can be decoupled at the cost of becoming second order, to yield the homogeneous wave-equation

\[
\begin{align*}
\nabla \times (\nabla \times \mathbf{E}) &= -\mu \frac{\partial \mathbf{H}}{\partial t} \\
-\nabla^2 \mathbf{E} + \nabla (\nabla \cdot \mathbf{E}) &= -\mu \varepsilon \frac{\partial}{\partial t} (\nabla \times \mathbf{H}) \\
\nabla^2 \mathbf{E} - \mu \varepsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} &= 0
\end{align*}
\]

In a similar way an identical equation for \( \mathbf{H} \) can be derived.

2.2 Scalar wave equation & paraxial optics

The vector wave equation as given in (7) will hold for all components of the \( E \) and \( H \) field individually and was derived for a linear, homogeneous, isotropic medium. This condition effectively rules out any
coupling between components, providing a means of simplifying the analysis. Of course, in the vicinity of any object, this condition of homogeneity is not satisfied. It is easily shown[3] how an inhomogeneous medium introduces coupling, by using a spatially dependent, non-zero permittivity \( \epsilon(r) \). The vector wave equation then becomes

\[
\nabla \times (\nabla \times E) = -\frac{\partial B}{\partial t} \\
-\nabla^2 E + \nabla(\nabla \cdot E) = -\mu \epsilon \frac{\partial}{\partial t}(\nabla \times B) \\
\n\nabla^2 E - \nabla(\nabla \cdot E) - \mu \epsilon \frac{\partial^2 E}{\partial t^2} = 0
\]

(8)

Note that \( \nabla \cdot E \) doesn’t vanish here because \( \epsilon \) is not constant. Using Maxwell’s equations we can write:

\[
\nabla \cdot \epsilon(r)E = E \nabla \epsilon(r) + \epsilon(r) \nabla \cdot E = 0 \\
-\frac{1}{\epsilon(r)} E \cdot \nabla \epsilon(r) = \nabla \cdot E
\]

(9)

(10)

Combining (9) and (10) then gives a vector wave equation again:

\[
\nabla^2 E + \nabla\left(\frac{1}{\epsilon(r)} E \nabla \epsilon(r)\right) - \mu \epsilon(r) \frac{\partial^2 E}{\partial t^2} = 0
\]

(11)

However, there is now coupling between the various components. Similar coupling originates when the medium is anisotropic or non-linear. When these conditions do hold however, there is no coupling and instead of all components we can write a scalar wave equation

\[
\left(\nabla^2 - \mu \epsilon \frac{\partial^2}{\partial t^2}\right) \Psi = 0
\]

(12)

where \( \Psi \) now denotes an arbitrary component. This simplification is common in scalar diffraction theory but the conditions imposed do limit how close to the aperture the field can be described; the condition of homogeneity clearly does not hold near a dielectric interface.

An additional simplification can be made by going to the paraxial approximation: the beams studied generally have a much smaller transversal extent than their distance of propagation. For monochromatic fields we can then write

\[
U(r,t) = \Psi(r)e^{-i\omega t}
\]

When this solution is substituted in (12), the Helmholtz equation is obtained:

\[
(\nabla^2 + k^2) \Psi = 0
\]

(13)

where \( k^2 = \mu \epsilon \omega^2 = (2\pi/\lambda)^2 \) is the wavenumber, and \( \lambda \) the wavelength. When the optical field \( \Psi(r) \) is propagated we are most interested in the transversal component of the field along the optical axis. Thus, if we align the optical axis along \( z \), we can model the dependence of the field as
\[ \Psi(x, y, z, t) = \psi(x, y, z)e^{ikz} \]  

(14)

The difference with a plane wave is that the amplitude of the field here is not a constant. Substituting (14) in (13) and simplifying then gives

\[ \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + 2ik \frac{\partial \psi}{\partial z} = 0 \]  

(15)

Under the assumption that the modulation, compared to the wavelength, is a slowly varying function of \( z \), we have

\[ \left| \frac{\partial^2 \psi}{\partial z^2} \right| \ll k \left| \frac{\partial \psi}{\partial z} \right| \]  

(16)

and the Helmholtz equation reduces to the paraxial Helmholtz equation

\[ \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + 2ik \frac{\partial \psi}{\partial z} = 0 \]  

(17)

### 2.3 Gaussian beams

A basis of solutions for the paraxial Helmholtz equation (17) can be shown [4, 3] to be Gaussian modes. The TEM\(_{00}\) mode is such as

\[ \Psi(x, y, z) = \frac{w(z)}{w(0)}e^{-\frac{x^2+y^2}{w(z)^2}}e^{-ik\left(\frac{x^2+y^2}{2w(z)^2}\right) + i\phi(z)}e^{ikz} \]  

(18)

which is referred to as a the fundamental Gaussian mode and it is of particular interest here for two reasons: it is the strongest order usually produced by the laser and it corresponds, to good approximation, to the transmission of a single-mode optical fiber. The functions \( w, R \) and \( \phi \) in (18) are respectively referred to as the beam waist, radius of curvature and the Gouy phase shift and are defined as

\[ w(z) = w_0 \sqrt{1 + \left(\frac{z}{z_R}\right)^2} \]  

(19)

\[ R(z) = z(1 + \frac{z^2}{z_R^2}) \]  

(20)

\[ \phi(z) = \arctan\left(\frac{z}{z_R}\right) \]  

(21)

Here, \( w_0 \) is the minimum beam waist, which is defined to be the point where the intensity of the beam has dropped to \( 1/e^2 \) of its maximum and \( z_R = \frac{\pi w_0^2}{\lambda} \) the Rayleigh length. As can be seen from (18), the beam has a transverse intensity profile that is a Gaussian:

\[ I(x, y, z) = |\Psi|^2 = \frac{w(z)^2 e^{-2(x^2+y^2)/w(z)^2}}{w(0)^2} = \frac{2P}{\pi w(z)^2} e^{-2(x^2+y^2)/(w(z)^2)} \]  

(22)

and the minimum beam waist is attained in the focus at \( z = 0 \). The divergence of the beam is often characterised by the far-field angle, that is is found to be
\[
\theta_F = \lim_{z \to \infty} \arctan \frac{w(z)}{z} \approx \frac{\lambda}{w_0 \pi}
\]  

It is intuitively clear from (23) that the more tightly focused the beam (smaller \(w_0\)), the larger the divergence (large \(\theta_F\)).

3. Diffraction effects

3.1 Power loss at edge

Given the beam intensity as in (22) and the waist as (19), it is clear from the geometry that part of the beam is truncated by the chip. The fraction of intensity that is not absorbed can be derived as a function of the the distance between the chip and optical axis \(d\), the beam waist at the focus \(w_0\) and the location of the focus with respect to the edge of the chip \(z_a\) to be:

\[
\frac{P_{\text{beam}}}{P_{\text{total}}} = \frac{1}{\mathcal{P}} \int_{-\infty}^{d} \int_{-\infty}^{\infty} \frac{2P}{\pi w(z_a)^2} e^{-\frac{x^2 + y^2}{w(z_a)^2}} dxdy
\]

\[
= \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{\sqrt{2}d}{w(z_a)} \right) \right]
\]

Since most of the geometry is fixed in this respect, the parameters to vary here are the beam waist and separation between the chip and the optical axis. Note that ideally, the latter is arranged to intersect with the cold gas and is thus not completely free to choose.

In figure (3) the calculated fractional energy loss from reflection off the chip is shown. It can be seen that the fractional energy loss has a minimum. This is the case when

\[
\frac{d}{dw_0} \left( \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{\sqrt{2}d}{w(z_a)} \right) \right] \right) = 0
\]

This expression can be solved analytically\(^1\) and yields a value for the 'optimum beam waist':

\[
w_0 = \sqrt{\frac{z_a \lambda}{\pi}}
\]

In the case \((z_a = 12.5 \text{ mm}, \lambda = 780 \text{ nm})\) we obtain \(w_0 \approx 55.7 \mu\text{m}\). Of course 'optimum' here refers to minimising the total energy loss: if one is simply interested in obtaining a very high intensity in a small focus then naturally a different beam waist will be required (even if cutting of part of the beam).

\(^1\)For derivation see appendix 2
Figure 3: Fractional energy loss (logarithmic scale) of beam impinging on a chip as a function of the beam waist $w_0$ at $z = 12.5$ mm for different separations ($d$) between the chip and optical axis.
3.2 Scalar diffraction theory

Diffraction is the phenomenon of the bending of waves around obstacles. This effect can be quantitatively explained by the Huygens-Fresnel principle, which describes the propagation of any wave in terms of the propagation of spherical waves originating at each point on the wavefront. Thus, any wave can be calculated by simply forward-propagating these point sources.

Figure 4: Geometry for Kirchhoff diffraction. $x_s$ denotes the source point. Image adapted from [13]

The mathematical theory of finding the wave amplitude at any point in space, given the wave at an arbitrary surface surrounding it was established by Kirchhoff, who expressed the field at any point in space $x_0$ in terms of the boundary values on a closed surface surrounding this point:

$$\Psi(x_0) = \iint_S \left[ \frac{\partial \Psi(x)}{\partial n} G(x) - \Psi(x) \frac{\partial G}{\partial n} \right] ds$$  \hspace{1cm} (28)

Here $G(x)$ is the Green’s function of the problem: a spherical wave expanding from the point $x_0$. To study diffraction from a planar aperture, Kirchhoff and Sommerfeld simplified the problem by segmenting the surface $S$ into parts $A$, $B$ and $C$, as shown in figure (4). Then given the conditions that the field on $A$ is identical to that without the screen and the field on $B$ and $C$ vanish$^2$, the integral reduces to the more familiar Kirchhoff-Sommerfeld diffraction integral:

$$\Psi(x, y, z) = \frac{1}{i\lambda} \iint_{-\infty}^{+\infty} \Psi(x', y', 0) e^{-ikr} \frac{\cos \theta dx' dy'}{r}$$  \hspace{1cm} (29)

Where $\lambda$ is the wavelength of the beam, $\theta$ the angle between the plane of diffraction and the observation direction and $r^2 = (x-x')^2 + (y-y')^2 + z^2$. The integral, being a solution to the homogenous wave equation under these boundary conditions, can be used to propagate waves from an aperture. Expressing $\cos \theta = z/r$ and taking terms in the integral we obtain

$^2$The latter condition is referred to as the Sommerfeld radiation condition [3, 9]
\[
\Psi(x, y, z) = \int \int_{-\infty}^{+\infty} \Psi(x', y', 0) e^{\frac{-i k z}{i \lambda z} \sqrt{1 + \frac{(x-x')^2}{z^2} + \frac{(y-y')^2}{z^2}}} dx' dy' \quad (30)
\]

There are two common approximations of this integral in the paraxial regime. One can do a binomial expansion on the square root and replace all occurrences in (30) with any number of terms:

\[
\sqrt{1 + \left(\frac{(x-x')^2}{z^2} + \frac{(y-y')^2}{z^2}\right)} \approx 1 + \frac{(x-x')^2}{2z^2} + \frac{(y-y')^2}{2z^2} - \frac{(x-x')^4}{8z^4} - \frac{(y-y')^4}{8z^4} + \cdots \quad (31)
\]

In the denominator, the error that results from dropping all terms but the constant is comparatively very small. In the exponential function, on the contrary, even a small phase shift can account for a large error, even more so because the value for \( k \) is typically very large in the optical regime (\( k \approx 10^7 \text{m}^{-1} \)). The **Fresnel** approximation is then obtained by keeping the second order terms in (31) only in the exponential, such that:

\[
\Psi(x, y, z) = \frac{e^{-ik z}}{i \lambda z} \int \int_{-\infty}^{+\infty} \Psi(x', y', 0) e^{-i k \left(\frac{(x-x')^2}{2z^2} + \frac{(y-y')^2}{2z^2}\right)} dx' dy' \quad (32)
\]

We can then expand the quadratic terms in the exponential

\[
\frac{(x-x')^2}{2z^2} + \frac{(y-y')^2}{2z^2} = \frac{x^2}{2z} - \frac{xx'}{z} + \frac{x'^2}{2z} + \frac{y^2}{2z} - \frac{yy'}{z} + \frac{y'^2}{2z} \quad (33)
\]

and take some of them outside the integral

\[
\Psi(x, y, z) = \frac{e^{-ik z}}{i \lambda z} e^{-i \frac{k}{2z}(x^2+y^2)} \int \int_{-\infty}^{+\infty} \Psi(x', y', 0) e^{i \frac{k}{2z}(x'^2+y'^2)} e^{-i \frac{k}{2z}(x'x+y'y')} dx' dy' \quad (34)
\]

Then under the additional Fraunhofer condition that, within the aperture

\[
z \gg \frac{k(x'^2+y'^2)}{2} \quad (35)
\]

the quadratic phase factor reduces to unity and the Fresnel integral (32) becomes the simpler **Fraunhofer** approximation:

\[
\Psi(x, y, z) = \frac{e^{-ik z}}{i \lambda z} e^{-i \frac{k}{2z}(x^2+y^2)} \int \int_{-\infty}^{+\infty} \Psi(x', y', 0) e^{-i \frac{k}{2z}(x'x+y'y')} dx' dy' \quad (36)
\]
Figure 5: Calculated diffraction intensity patterns for a plane wave ($\lambda = 780 \text{ nm}$) incident on a rectangular aperture ($D = 0.2 \text{ mm}$) at different distances from the aperture. Fresnel numbers separating the reactive, Fresnel and Fraunhofer regime are shown along the propagation axis.

Now the different regimes described are valid in certain regions behind the aperture. According to [3] these regions can be characterised by the Fresnel number, which provides a practical means of deciding which regime is relevant. The Fresnel number is a dimensionless value defined as:

$$F = \frac{D^2}{\lambda z}$$

Here, $D$ is the aperture size and $\lambda$ and $z$ are the wavelength and distance from the aperture respectively. In line of the discussion above, the Fresnel number can be used to distinguish between the different diffraction regimes as follows:

1. Reactive near-field: $F \gg 1$ (Kirchhoff when $z > \lambda/2$, otherwise other approach)
2. Radiative near-field: $F \simeq 1$ (Fresnel integral)
3. Far-field: $F \ll 1$ (Fraunhofer integral)

As a test of the numerical propagation (see next section), diffraction patterns for the well known case of a plane wave ($\lambda = 780 \text{ nm}$) incident on a square aperture ($D = 0.2 \text{ mm}$) were calculated using scalar diffraction theory and are shown in figure (5). For the geometry described in the first section, the Fresnel number is of the order $\approx 10^9$: clearly either in the reactive near-field or radiative near-field. The Fraunhofer approximation is thus of no relevance for the intensity pattern in the region of the gas.

### 3.3 Numerical modelling of diffraction

Analytical solutions to the diffraction equations are generally not available except for very simple geometries. In effect, one has to resort to numerical techniques for solving these equations. One
convenient way of viewing diffraction is as a convolution with a diffraction kernel (sometimes referred to as a transfer function). Recalling the definition of a convolution of functions:

\[ f \ast g = \int f(x)g(x-x')dx' \]

We can write the Rayleigh-Sommerfeld diffraction integral simply as a convolution of the aperture function with a diffraction kernel:

\[ \Psi(x, y, z) = \Psi(x', y', 0) \ast h(x, y, z) \]

where the diffraction kernel in this case is

\[ h(x, y, z) = \frac{e^{ikz\sqrt{1 + \frac{x^2}{z^2} + \frac{y^2}{z^2}}}}{i\lambda z \left(1 + \frac{x^2}{z^2} + \frac{y^2}{z^2}\right)} \]

A convolution is easily performed in the Fourier-transformed domain, where the convolution of two functions is simply the product of Fourier-transforms. The optical field \( \Psi(x, y, z) \) can thus be found by taking

\[ \Psi(x, y, z) = \mathcal{F}^{-1} \left[ \mathcal{F} \left[ \Psi(x', y', 0) \ast h(x, y, z) \right] \right] \]

\[ = \mathcal{F}^{-1} \left[ \mathcal{F} \left[ \Psi(x', y', 0) \right] \cdot \mathcal{F} \left[ h(x, y, z) \right] \right] \tag{37} \]

\[ = \mathcal{F}^{-1} \left[ \mathcal{F} \left[ \Psi(x', y', 0) \right] \right] \cdot \mathcal{F} \left[ h(x, y, z) \right] \tag{38} \]

Where the Fourier-transform of \( h(x, y, z) \) can be done analytically, to yield the transfer function:

\[ \mathcal{F} \left[ h(x, y, z) \right] = H(p, q) = e^{-ikz\sqrt{1 - \lambda^2(p^2 + q^2)}} \]

Doing diffraction in the Fourier-transformed domain has the advantage that it can be performed relatively quickly using Fast-Fourier Transforms in mathematical packages such as MATLAB. In fact, for long one dimensional convolutions with \( N \) samples in the discrete domain, the number of operations performed grows as \( N^2 \) while the number of operations for FFT grows as \( N \log_2 N \) [10]. Performance comparison between the two methods was done in MATLAB by repeating one operation many times and then averaging the computation time. In the 2D domain then, where we generally have samples of size \( N^2 \), it is clear that the improved computation time is much more pronounced.
Figure 6: Time per operation in ms for 1D direct convolution of a N-sized sample compared to using FFT in MATLAB 7.12 on Intel 2.5 GHz Windows PC.

The performance of (38) is determined by two factors: the sampling rate and the domain. While the latter is determined by the spatial extent of the beam over the diffraction distance, the sampling rate is largely determined by the wavelength involved. According to the Shannon-Nyquist sampling theorem, to avoid aliasing of a signal of frequency \( f \), the minimum sampling rate needs to be at least \( 1/2f \). In the case of a laser with \( \lambda = 780 \) nm this puts a lower limit on the resolution of 390 nm/pixel. For a reasonable geometry where the aperture and focus are separated by 10 mm and a beam waist of 10 \( \mu \)m in the focus, the width is already on the order of 250 \( \mu \)m at the aperture. To avoid edge effects with the Fourier Transform, the boundaries of the computational domain must necessarily be zero, therefore, the domain needs to be several times the waist to ensure this. Given a sampling rate of 390 nm/pixel this means that for a 2D diffraction, \( N \) is already on the order of \( 10^6 \). In addition to the large domain, FFT requires computational domains that are integers powers of 2, and if this is not the case it will simply extend the domain to the nearest power of 2.

It is clear that a faster way would be to split the integral. In the particular case of a beam cut by a half plane this is possible since the step-function used in the x-direction, is also symmetrical about \( y = 0 \). Thus, starting from the Fresnel approximation to the Kirchhoff-Fresnel diffraction integral (29):

\[
\Psi(x, y, z) = \frac{e^{ikz}}{i\lambda z} \int_{-\infty}^{+\infty} \Psi(x', y', 0) e^{ik\left(\frac{(x-x')^2}{4z} + \frac{(y-y')^2}{4z}\right)} dx' dy' \tag{39}
\]

The optical field \( \Psi(x', y', 0) \) in this case is a Gaussian beam multiplied by a Heaviside function that is shifted from the origin:

\[
\Psi(x, y, z) = \Psi_{LASER} H(d - x) \tag{40}
\]

Both the Fresnel integral and incident field are separable, that is they can be written as a product of functions of \( x, y \) and \( z \)

\[
\Psi_{LASER}(x, y, z) = \frac{w(z)}{w(0)} e^{ikz} e^{ik\phi(z)} e^{-\frac{x^2}{w(z)^2}} e^{-\frac{y^2}{w(z)^2}} e^{-ik\left(\frac{x'^2}{4z} + \frac{y'^2}{4z}\right)} \tag{41}
\]
\[ \Psi_L^x \Psi_L^y \Psi_L^z \] (42)

where we denote

\[ \Psi_L^x = e^{-\frac{x'^2}{2w(x)^2}} e^{-ik\frac{x'^2}{2R(z)}} \]
\[ \Psi_L^y = e^{-\frac{y'^2}{2w(y)^2}} e^{-ik\frac{y'^2}{2R(z)}} \]
\[ \Psi_L^z = \frac{w(z')}{w(0)} e^{ikz} e^{ik\phi(z)} \]

such that the integral becomes

\[ \Psi(x, y, z) = \frac{e^{ikz}}{i\lambda z} \Psi_L^z \int \Psi_L^x e^{ik\frac{(x-x')^2}{2z}} H(d-x')dx' \int \Psi_L^y e^{ik\frac{(y-y')^2}{2z}} dy' \]

Thus, 2D diffraction can be performed by simply doing 1D diffraction integrals, which yields a substantial performance enhancement.

### 3.4 Beam diffraction patterns

Both 1D and 2D discrete versions of diffraction integrals were programmed in MATLAB to calculate beam propagation. Grid resolution was chosen to satisfy the Nyquist-Shannen minimum sampling rate. Transverse cross-sections of the beam intensity at different distances from the aperture are shown in figure (7). The Fresnel patterns are clearly visible close to the aperture. In addition, cross-sections along the \( y = 0 \) axis are shown in figure (8). Propagation with different parameters was performed and can be found in appendix 3.

![Figure 7: Transverse beam crossections at (left to right) \( z = 2.5 \text{ mm}, 7.5 \text{ mm}, 12.5 \text{ mm} \) where \( w_0 = 20 \mu \text{m} \) and \( d = 50 \mu \text{m} \) with the focus in \( z = 12.5 \text{ mm} \). Interference fringes are clearly visible near the aperture.](image)

In all cases, the perturbation of the field near the focus is minimal and the beam develops a smooth Gaussian-like shape, be it with a displaced center. For different values of \( d \) the displacement of the beam center with respect to the optical axis was calculated by fitting the curve to a Gaussian. The result is shown, in figure (17), along with later results (in section 4.5).
4. Reflection from the atom chip

The model described in section 3 can be used to calculate diffraction by a half-plane without the chip surface being present. In the setup however, in addition to being diffracted by the edge, part of the beam will be incident on the chip surface. When light hits an interface between two materials with different refractive indices, both reflection and transmission can occur. In addition to the normal diffracted field, a more accurate model also needs to take this reflection into account. It is clear from figure 7 and (8) that this is not currently the case, as there is field intensity in the chip region.

Our current model can be adapted for reflections by viewing the diffraction integral (29) as a propagation of paraxial plane waves, each with a different amplitude and angle with respect to the optical axis. This method is commonly\[3, 16\] used for propagation of fields when effects like attenuation, refraction and reflection need to be considered. The advantage of decomposing the field into plane waves is that plane waves are theoretically and intuitively much easier objects and, in our particular case, Fresnel coefficients for plane waves are readily determined\[5, 7\]. The method can be divided into several steps, that will be treated in detail in the sections below:

1. Sampling of a cross-section of the beam at a particular \( z = z_0 \). In the case of an atom chip, the most natural position is the edge of the chip where the field is cut off.

2. Decomposition of the beam into it’s angular spectrum: this will result in a set of plane wave components.

3. Propagate each individual plane wave to the plane of interest by multiplying each component with a phase shift factor. In the case of reflection, both an non-trivial phase shift factor and Fresnel coefficient needs to be taken into account.

4. Recover the field at the plane of interest by doing an inverse transformation.
4.1 Angular decomposition

To derive the plane wave decomposition (largely following [4]) of the beam, we start with the expression for a general plane wave:

$$\psi(x, y, z) = e^{i(k_x x + k_y y + k_z z)}$$

Where \( k \) is the propagation vector. If the angles with the \( x \), and \( y \) axes are respectively \( \theta_x \) and \( \theta_y \), then we can write

$$\psi(x, y, z) \approx e^{i(k_x \sin \theta_x x + k_y \sin \theta_y y + \sqrt{k^2 - k_x^2 - k_y^2} z)}$$

$$\approx e^{i(k_x \sin \theta_x x + k_y \sin \theta_y y) + i(k - \pi \lambda (s_x^2 + s_y^2)) z}$$

where \( 2\pi s_x = k \sin \theta_x \), \( 2\pi s_y = k \sin \theta_y \). Any field \( \Psi(x, y, z) \) can then be decomposed into plane waves as

$$\Psi(x, y, z) = \int \int \hat{\Psi}(s_x, s_y, 0) \psi(x, y, z) ds_x ds_y$$

$$\approx \int \int \hat{\Psi}(s_x, s_y, z) e^{i(2\pi s_x x + 2\pi s_y y) + i(k - \pi \lambda (s_x^2 + s_y^2)) z} ds_x ds_y$$

where \( \hat{\Psi}(s_x, s_y, 0) \) is the angular spectrum. At an arbitrary plane \( z_0 \) the beam is given by

$$\Psi(x, y, z_0) = \int \int \hat{\Psi}(s_x, s_y, z_0) e^{i(2\pi s_x x + 2\pi s_y y)} ds_x ds_y$$

(43)

And the angular distribution \( \hat{\Psi}(s_x, s_y, z_0) \) is found by taking the inverse Fourier transform:

$$\hat{\Psi}(s_x, s_y, z_0) = \int \int \Psi(x, y, z_0) e^{-i(2\pi s_x x + 2\pi s_y y)} dx dy$$

4.2 Propagation in the angular domain

Propagation in the angular domain from plane \( z = z_0 \) to \( z = z \) is simply performed by multiplying the angular distribution by the phase shift factor

$$\hat{\Psi}(s_x, s_y, z) = \hat{\Psi}(s_x, s_y, z_0) e^{i(k(z - z_0) - \pi \lambda (s_x^2 + s_y^2)(z - z_0))}$$

(44)

The field distribution is then recovered by an inverse transformation as in (43). This phase shift factor can be derived both from theoretical considerations or a geometric argument. The first is done in appendix 4.
Figure 9: Geometry for determining the phase shift. Here $L$ is the distance the plane wave originating in $z = z_0$ will have travelled when reaching the plane of interest.

while for the latter we will use figure (9) to derive it. Here, the phase shift factor acquired by the beam by moving from $z = z_0$ to $z = z$ is given as

$$e^{ikL} = e^{i\frac{2\pi}{\lambda}(z-z_0) \cos \theta_y \cos \theta_x} = e^{i\frac{2\pi}{\lambda}(z-z_0)(1-\theta_y^2)(1-\theta_x^2)} \approx e^{ik(z-z_0)} e^{-i\pi \lambda(x^2 + y^2)(z-z_0)} \quad (45)$$

where use was made of the second order approximation of the cosine, and combinations $\theta_y^2 \theta_x^2$ were discarded. An example of propagation in the angular domain is shown in figure (10), where a Gaussian beam is propagated in the angular domain to different distances. If reflection is to be taken into account, apart from the angular spectrum that propagates normally, there is an additional set of waves that is phase-shifted and possibly transformed by the reflecting surface. This transformation depends both on the nature of the dielectric and the angle of incidence, and is quantitatively determined by the Fresnel equations. These relate the incoming amplitude and phase to the reflected/transmitted amplitude and phase.

Figure 10: Real part of a Gaussian beam with $w_0 = 1$ mm and $\lambda = 0.2$ mm propagated in the angular domain. The large wavelength was chosen purely for illustrative purposes.

The angles of reflection $\theta_R$ and transmission $\theta_T$ of a plane wave at an interface are determined by Snell’s law:
\[
\frac{\sin \theta_T}{\sin \theta_I} = \frac{n_1}{\tilde{n}} \quad \theta_I = \theta_R
\]

with \( \tilde{n}, n_1 \) the (complex) refractive index of the medium and the angles as given in figure (11).

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{interface.png}
\caption{Interface}
\end{figure}

And the Fresnel reflection coefficients depend on the polarisation of the light and the incoming angle and can be derived from Maxwell’s equation ³. For simplicity we will consider only s-polarized waves (where the polarization is perpendicular to the plane of incidence):

\[
\Psi_R = \left( \frac{1 - \alpha \tilde{\beta}}{1 + \alpha \tilde{\beta}} \right) \Psi
\]

where the constants \( \alpha \) and \( \tilde{\beta} \) are defined as

\[
\tilde{\beta} = \frac{\mu_1 \tilde{n}}{\mu_2 \tilde{n}} \\
\alpha = \frac{\cos \theta_T}{\cos \theta_I} = \sqrt{1 - \left( \frac{n_1}{n} \right)^2 \sin^2 \theta_i}
\]

Now the phase shift of this reflected wave is not easily determined but can be derived with help of figure (12). The distance of any plane wave to the plane of interest \( z = z_0 \) is composed of three parts, \( L_1, L_2 \) and \( L_3 \), for which expressions can be found:

³See appendix 1 for a complete derivation
Figure 12: Reflection geometry

\[ L_1 = \sin \theta \left( 2d - z' \tan \theta \right) \simeq 2d \theta - z' \theta_x^2 \]

\[ L_2 = \frac{z' - \frac{d}{\cos \theta_x}}{\tan \theta_x} \simeq -\frac{d}{\theta_x} + z' - \frac{d \theta_x}{6} + \frac{z \theta_x^2}{2} \]

\[ L_3 = \frac{d}{\sin \theta_x} \simeq \frac{d}{\theta_x} \]

where \( z' = z_0 \cos \theta_y \). The small angle, second order approximations can be made plausible by realising we’re in the paraxial regime, where by definition the deviation from the optical axis is very small. To propagate the angular spectrum then, an additional phase shift of

\[ e^{ik(L_1+L_2+L_3)} \simeq e^{ikz_0}e^{-ik\left(\frac{z_0 \theta_x^2}{2} + \frac{z \theta_x^2}{2}\right)e^{ikd\theta_x}} \]

has to be included. The wave at position \( z \) can then be reconstructed by summing the normal propagating part (44) and the reflected part, taking into account the reflection coefficients (and the change of direction of the beam due to reflection):

\[ \tilde{\Psi}(s_x, s_y, z) = \tilde{\Psi}(s_x, s_y, z_0)e^{ikz_0}e^{-ik\left(\frac{z_0 \theta_x^2}{2} + \frac{z \theta_x^2}{2}\right)e^{ikd\theta_x}} \left( \frac{1 - \alpha \beta}{1 + \alpha \beta} \right) \]

Note that, while not mentioned, \( \alpha \) too is a function of \( \theta_x \) here. Care must be taken if the chip is of finite extent, for portions of the angular spectrum might not be reflected at all. In the present case, where all angles are very small and the reflectivity is very high, we can model the chip as a perfect conductor. It is redundant in that case to use the full power of the angular decomposition, and it suffices to simply back-reflect, in real space, the part of the diffracted electric field occupying the chip region. This has the additional advantage that beam propagation in real space requires less complex sampling conditions: in the angular domain however, care must be taken to prevent aliasing from the quadratic phase factors, as described in [17].

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4.3 Fresnel coefficients of gold

Using the complex refractive index for gold at 780 nm from [15], both phase and amplitude of the reflection coefficient can be determined from (46) as a function of the angle of incidence. The result is shown in figure (13).

Figure 13: Amplitude (left) and phase (right) of Fresnel reflection coefficient of gold for parallel (dotted) and perpendicular (solid) polarization at 780 nm between 0-20°. Inset: coefficients between 0-90°.

4.4 Fresnel coefficients for silicon monocrystals

Using the complex refractive index for silicon monocrystals at 780 nm from [14], both phase and amplitude of reflection coefficient can be determined from (46) as a function of incidence angle. The result is shown in figure (14).

Figure 14: Amplitude (left) and phase (right) of Fresnel reflection coefficient of silicon monocrystal for parallel and perpendicular polarization at 780 nm between 0-20°. Inset: coefficients between 0-90°.
4.5 Beam diffraction and reflection

Beam propagation was performed in the 1D-regime, where a beam with focus at $z = 12.5$ mm, beam waist $w_0 = 50 \mu m$ and $d = 50 \mu m$ was propagated using both the model with Fresnel coefficients and the simplified model using a $180^\circ$ phase shift and back-reflection in real space. While in the latter method the field at the boundary of the chip was 0, a small remnant field remained in the more accurate model, yet no large deviations between the two methods was seen. This is as expected, for gold was chosen for being a near-perfect reflector for beams with wavelengths in the IR regime. Beams were propagated to $z = 2.0$ mm and $z = 12.5$ mm to show the effect of diffraction: closer to the aperture interference fringes are seen in both the reflected and diffracted beam, while far from the edge the field is smooth.

![Cross-section of beam propagated to $z = 2.0$ mm, focus at $z = 12.5$ mm, beam waist $w_0 = 50 \mu m$ and $d = 50 \mu m$. Shown are both the diffracted beam and the one with reflection included.](image)

Figure 15: Cross-section of beam propagated to $z = 2.0$ mm, focus at $z = 12.5$ mm, beam waist $w_0 = 50 \mu m$ and $d = 50 \mu m$. Shown are both the diffracted beam and the one with reflection included.
Figure 16: Cross-section of beam propagated to \( z = 12.5 \text{ mm} \), focus at \( z = 12.5 \text{ mm} \), beam waist \( w_0 = 50 \mu\text{m} \) and \( d = 50 \mu\text{m} \). Shown are both the diffracted beam and the one with reflection included.

As visible in (15),(16), diffraction and reflection causes the beam maximum to be displaced from the optical axis. To determine the size of the displacement, the both beams were fitted to a Gaussian distribution for different distances between the optical axis and chip. The results are shown in figure (17).

Figure 17: Displacement of the beam maximum, found by propagating the beam up to \( z = 12.5 \text{ mm} \), including reflection and fitting the resulting curve to a Gaussian.

5. Time-domain simulation: a viability study

While beam reflection can now be taken into account, there is no trivial way to adapt the diffraction integrals or angular spectrum method to include diffraction effects from on-chip wires or objects sur-
rounding the chip, while it is known that such objects alter the field. To take these into account, a more general method is required. Finite-Difference Time-Domain (FDTD) is such a numerical method for performing computational electrodynamics in the time domain. It is a full-wave method of solving Maxwell’s equations directly and can therefore solve much more general electrodynamics problems, at the cost of being computationally much more expensive than diffraction integrals. The FDTD method uses finite differences as approximations to the derivatives in Maxwell’s equation. Using a Taylor expansion of \( f(x) \) about the point \( x_0 \) at \( x_0 + \frac{\delta}{2} \) then gives

\[
\begin{align*}
  f(x_0 + \frac{\delta}{2}) &= f(x_0) + \frac{\delta}{2} f'(x_0) + \frac{1}{2!} \left( \frac{\delta}{2} \right)^2 f''(x_0) + \frac{1}{3!} \left( \frac{\delta}{2} \right)^3 f'''(x_0) + \cdots \quad (47) \\
  f(x_0 - \frac{\delta}{2}) &= f(x_0) - \frac{\delta}{2} f'(x_0) + \frac{1}{2!} \left( \frac{\delta}{2} \right)^2 f''(x_0) - \frac{1}{3!} \left( \frac{\delta}{2} \right)^3 f'''(x_0) + \cdots \quad (48)
\end{align*}
\]

Now subtracting (47) from (48) yields

\[
\begin{align*}
  f(x_0 + \frac{\delta}{2}) - f(x_0 - \frac{\delta}{2}) &= \delta f'(x_0) + \frac{2}{3} \left( \frac{\delta}{2} \right)^3 f'''(x_0) + \cdots \quad (49)
\end{align*}
\]

Or, in a more convenient form

\[
\begin{align*}
  f'(x_0) &= \frac{f(x_0 + \frac{\delta}{2}) - f(x_0 - \frac{\delta}{2})}{\delta} + \frac{1}{3!} \left( \frac{\delta}{2} \right)^2 f'''(x_0) + \cdots \quad (50) \\
  &= \frac{f(x_0 + \frac{\delta}{2}) - f(x_0 - \frac{\delta}{2})}{\delta} + O(\delta^2) \quad (51)
\end{align*}
\]

FDTD now works by discretizing space and time and replacing all derivatives in Maxwell’s coupled equations with the finite difference approximations.

![Yee Cube: the discretization of space](image)

**Figure 18:** Yee Cube: the discretization of space

The discretization of space is done using a Yee cube, shown in figure (18), where one should note that the components of \( E \) and \( H \) are spatially offset from each other. In addition to this spatial offset, the \( E \) and \( H \) fields are also offset in time, and the propagation algorithm works by progressively...
calculating one field from another by means of update equations. Since the 2D/3D case is particulary
tedious to handle: consider the one dimensional case in which the electric field has a z-component only.
In that case Maxwell’s vector equations reduce to two scalar coupled equations in \( E_z \) and \( H_y \)
\[
\frac{\mu}{\epsilon} \frac{\partial H_y}{\partial t} = \frac{\partial E_z}{\partial x} \tag{52}
\]
\[
\epsilon \frac{\partial E_z}{\partial t} = \frac{\partial H_y}{\partial x} \tag{53}
\]
Now discretization means the \( E \) and \( H \) components are sampled at discrete time and space intervals.
If the interval between space intervals is \( \Delta x \) and time intervals is \( \Delta t \) then using the Yee cube and the
difference approximation we can write the discretization of (53) as
\[
\frac{\epsilon E_z(n\Delta x, (t + 1)\Delta t) - E_z(n\Delta x, t\Delta t)}{\Delta t} = \frac{H_y((n + \frac{1}{2})\Delta x, (t + \frac{1}{2})\Delta t) - E_z((n - \frac{1}{2})\Delta x, (t + \frac{1}{2})\Delta t)}{\Delta x}
\]
Note that the \( H \)-field lags half a timestep behind the electric field and is displaced in space by exactly
the side of a Yee cube. This equation can be solved for \( E_z(n\Delta x, (t + 1)\Delta t) \) to give
\[
E_z(n\Delta x, (t + 1), t\Delta t) = E_z(n\Delta x, t\Delta t) + \frac{\Delta t}{\epsilon \Delta x} \left( H_y((n + \frac{1}{2})\Delta x, (t + \frac{1}{2})\Delta t) - E_z((n - \frac{1}{2})\Delta x, (t + \frac{1}{2})\Delta t) \right)
\]
A similar equation can be derived for the \( H \) field. These update equations can be used to progressively
step the the \( E \) and \( H \) fields, the accuracy largely determined by a choice of \( \frac{\Delta t}{\epsilon \Delta x} \). This ratio is
proportional to the Courant number, which is related to the stability of the simulation [11]. An
important other concern in doing FDTD calculations is the finite computational domain: because
of this finite domain eventually waves will reach the boundaries of the grid and will reflect. This is
a considerable problem, because computation time is closely linked to grid size and the smaller the
grid the more reflections from boundaries can be expected. To resolve this, artificial absorbing layers,
referred to as PML (Perfectly Matched Layer) , that will absorb any incoming waves at the interface
and thus prevent reflections are commonly used [18, 19].

To examine the feasibility of using FDTD simulation for diffraction problems near the atom chip,
use was made of MIT’s open FDTD simulation package MEEP[12]. FDTD simulation of a Gaussian
beam impinging on a conductor was performed. Due to the large computational domain required for
reasonable results (with a \( \lambda=780 \) nm, \( w_0 = 50 \mu m \)) and resulting large computation times, only the
(reactive) near field was examined for a small beam (\( w_0 = 5 \mu m \)). The computational domain was
chosen to be 500 \( \mu m \) by 80 \( \mu m \) with a resolution of 0.1 \( \mu m/pixel \) (or 10 pixels/\( \mu m \) alternatively). The
simulation was run for 800 timesteps, to eliminate any transient phenomena.

Identical analysis was performed for a plane wave incident on a rectangular aperture, yielding similar
results to the diffraction integral. While providing a general approach to solving diffraction from small
objects, computational time is a serious issue in FDTD analysis: for a realistic grid containing the
region of interest the calculation time already exceeded one hour.

6. Conclusions and outlook

A method for computing diffraction patterns from a Gaussian beam incident on a thick surface was
developed. To verify the validity of the diffraction patterns produced, other diffraction patterns for
geometries with analytical solutions (plane waves on a square aperture in the near- and far-field and Gaussian beams in the far field) were calculated with the same method and compared against the exact solution. With the exception of minor aliasing, which can be resolved by increasing the computational domain, there were no deviations found. Reflections can be included in the 1D regime using the model for a perfect reflector, as long as the incidence angles are small: this is guaranteed in the paraxial approximation, as long as the beam as a whole travels parallel to the chip surface. Similar results can be obtained using the angular spectrum method, yet a more detailed analysis is needed for the specific requirements for sampling in the angular domain. In conclusion, one can use the current software to calculate the effects of diffraction from an atom chip. FDTD computation was shown feasible, although substantial increase in computation time is expected for realistic grids that should extend over a range of 12500 µm. Although the method is significantly slower than diffraction integrals it has the added advantage of being able to include all beam polarizations and more complex chip geometry. Since it is known from experimental observations in the CELSIUS experiment that there is significant diffraction from small objects on the surface of the chip, a mixed method approach, where diffraction integrals are used to propagate the beam close to the gas followed by FDTD analysis in the small computational domain containing the region of interest, should be investigated.

Figure 19: FDTD simulation with Gaussian beam with λ = 0.78 µm. Propagation domain visible is 80 µm. The chip was modelled as perfect reflector. Beam waist at focus 5 µm. Resolution of simulation 0.1 µm/pixel. Computation time was 1 minute.
Bibliography


Appendix 1 - Fresnel coefficients for conductors

Maxwell’s equations in matter are

\[ \nabla \cdot \mathbf{D} = \sigma_f \]
\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \]  \hspace{1cm} (54)
\[ \nabla \cdot \mathbf{B} = 0 \]
\[ \nabla \times \mathbf{H} = \mathbf{J}_f + \frac{\partial \mathbf{D}}{\partial t} \]  \hspace{1cm} (55)

If any charges in the conductor are considered bound charges, then \( \sigma_f = 0 \), and thus \( \mathbf{J}_f = 0 \), so that the equations reduce to

\[ \nabla \cdot \mathbf{D} = 0 \]
\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \]  \hspace{1cm} (56)
\[ \nabla \cdot \mathbf{B} = 0 \]
\[ \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} \]  \hspace{1cm} (57)

Using approximation \( \mathbf{H} \approx \mathbf{B}/\mu_0 \) and applying the curl to (56) gives

\[ \nabla \times (\nabla \times \mathbf{E}) = -\frac{\partial \mathbf{B}}{\partial t} \]
\[ -\nabla^2 \mathbf{E} + \nabla (\nabla \cdot \mathbf{E}) = -\mu_0 \frac{\partial}{\partial t} (\nabla \times \mathbf{B}) \]
\[ \nabla^2 \mathbf{E} = \mu_0 \frac{\partial^2 \mathbf{D}}{\partial t^2} \]  \hspace{1cm} (58)

Looking at monochromatic waves \( \mathbf{E} = \mathbf{E}(r)e^{-i\omega t} \), under the assumption that \( \mathbf{D} = \tilde{\epsilon} \mathbf{E} \), where \( \tilde{\epsilon} \) is complex, this reduces to a differential equation for the spatial part of the E-field:

\[ \nabla^2 \mathbf{E}(r) = -\mu_0 \tilde{\epsilon} \omega^2 \mathbf{E}(r) \]  \hspace{1cm} (59)

The solutions to (58) are then plane waves, written as

\[ \mathbf{E}(r, t) = \mathbf{E}_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} \]  \hspace{1cm} (60)

with complex wavevector \( \mathbf{\tilde{k}} \) such that \( |\mathbf{\tilde{k}}| = \mathbf{\tilde{k}} = \sqrt{\mu_0 \tilde{\epsilon} \omega} \). The wave vector is related to the dielectric constant and refractive index by:

\[ \mathbf{\tilde{k}} = \omega \sqrt{\mu_0 \epsilon_0 \epsilon_r} = \frac{\omega \sqrt{\epsilon_r}}{c} \]  \hspace{1cm} (61)
\[ \tilde{n} \equiv \frac{c}{\omega \mathbf{k}} = \sqrt{\epsilon_r} \]  \hspace{1cm} (62)

Faraday’s law imposes an additional constraint on the fields, because
\[ \nabla \times \mathbf{E} = \begin{pmatrix} \hat{i}k_y E_z - \hat{i}k_z E_y \\ \hat{i}k_z E_x - \hat{i}k_y E_z \\ \hat{i}k_x E_y - \hat{i}k_y E_x \end{pmatrix} = \begin{pmatrix} i\omega B_x \\ i\omega B_y \\ i\omega B_z \end{pmatrix} \] (63)

This effectively means we can write \( \mathbf{B} \) in terms of \( \mathbf{E} \):

\[ \mathbf{B}(\mathbf{r}, t) = \frac{1}{\omega} \hat{k} \times \mathbf{E} \] (64)

Now suppose a plane wave in a medium with dielectric constant \( \epsilon_1 \), impinges on a medium with dielectric constant \( \tilde{\epsilon} \), as shown in figure (20).

![Figure 20: Interface](image)

The boundary conditions at the interface \( z = 0 \) are

\[ \epsilon_1 E_1^\perp - \tilde{\epsilon} E_2^\perp = 0 \] (65)
\[ B_1^\perp - B_2^\perp = 0 \] (66)
\[ E_1^\parallel - E_2^\parallel = 0 \] (67)
\[ \frac{1}{\mu_1} B_1^\parallel - \frac{1}{\mu_2} B_2^\parallel = 0 \] (68)

The direction of the wave vector can be written as:
\[ \hat{k}_I = \sin \theta_I \hat{x} + \cos \theta_I \hat{z} \quad \hat{k}_R = \sin \theta_R \hat{x} - \cos \theta_R \hat{z} \quad \hat{k} = \sin \theta_T \hat{x} + \cos \theta_T \hat{z} \]  

(69)

For incidence **perpendicular** to the plane of incidence, the fields then become (removing time-dependence and using (64))

\[
\begin{align*}
E_I & = E_{I,0} e^{i \mathbf{k}_1 \cdot \mathbf{r}} \hat{y} \\
B_I & = \frac{E_{I,0}}{v_1} (-\cos \theta_I \hat{x} + \sin \theta_I \hat{z}) e^{i \mathbf{k}_1 \cdot \mathbf{r}} \\
E_R & = E_{R,0} e^{i \mathbf{k}_R \cdot \mathbf{r}} \hat{y} \\
B_R & = \frac{E_{R,0}}{v_1} (\cos \theta_R \hat{x} + \sin \theta_R \hat{z}) e^{i \mathbf{k}_R \cdot \mathbf{r}} \\
E_T & = E_{T,0} e^{i \mathbf{k}_T \cdot \mathbf{r}} \hat{y} \\
B_T & = \frac{\hat{k}}{\omega} E_{T,0} (-\cos \theta_T \hat{x} + \sin \theta_T \hat{z}) e^{i \mathbf{k}_T \cdot \mathbf{r}}
\end{align*}
\]

While for incidence **parallel** to the plane of incidence, the fields are

\[
\begin{align*}
E_I & = E_{I,0} e^{i \mathbf{k}_1 \cdot \mathbf{r}} (-\sin \theta_I \hat{z} + \cos \theta_I \hat{x}) \\
B_I & = \frac{E_{I,0}}{v_1} e^{i \mathbf{k}_1 \cdot \mathbf{r}} \hat{y} \\
E_R & = E_{R,0} e^{i \mathbf{k}_R \cdot \mathbf{r}} (\sin \theta_R \hat{z} + \cos \theta_R \hat{x}) \\
B_R & = \frac{E_{R,0}}{v_1} e^{i \mathbf{k}_R \cdot \mathbf{r}} \hat{y} \\
E_T & = E_{T,0} e^{i \mathbf{k}_T \cdot \mathbf{r}} (-\sin \theta_T \hat{z} + \cos \theta_T \hat{x}) \\
B_T & = \frac{\hat{k}}{\omega} E_{T,0} e^{i \mathbf{k}_T \cdot \mathbf{r}} \hat{y}
\end{align*}
\]

For **perpendicular** polarization this yields a set of equations:

\[
\begin{align*}
\frac{E_{I,0}}{v_1} \sin \theta_I e^{i \mathbf{k}_1 \cdot \mathbf{r}} + \frac{E_{R,0}}{v_1} \sin \theta_R e^{i \mathbf{k}_R \cdot \mathbf{r}} & = \frac{\hat{k}}{\omega} E_{T,0} \sin \theta_T e^{i \mathbf{k}_T \cdot \mathbf{r}} \\
\frac{E_{I,0}}{v_1} e^{i \mathbf{k}_1 \cdot \mathbf{r}} + \frac{E_{R,0}}{v_1} e^{i \mathbf{k}_R \cdot \mathbf{r}} & = E_{T,0} e^{i \mathbf{k}_T \cdot \mathbf{r}} \\
\frac{1}{\mu_1} (-\frac{E_{I,0}}{v_1} \cos \theta_I e^{i \mathbf{k}_1 \cdot \mathbf{r}} + \frac{E_{R,0}}{v_1} \cos \theta_R e^{i \mathbf{k}_R \cdot \mathbf{r}}) & = -\frac{\hat{k}}{\mu_2 \omega} E_{T,0} \cos \theta_T e^{i \mathbf{k}_T \cdot \mathbf{r}}
\end{align*}
\]

While for **parallel** polarization it yields:

\[
\begin{align*}
\epsilon_1 (-E_{I,0} e^{i \mathbf{k}_1 \cdot \mathbf{r}} \sin \theta_I + E_{R,0} e^{i \mathbf{k}_R \cdot \mathbf{r}} \sin \theta_R) & = \epsilon (-E_{T,0} e^{i \mathbf{k}_T \cdot \mathbf{r}} \sin \theta_T) \\
E_{I,0} e^{i \mathbf{k}_1 \cdot \mathbf{r}} \cos \theta_I + E_{R,0} e^{i \mathbf{k}_R \cdot \mathbf{r}} \cos \theta_R & = E_{T,0} e^{i \mathbf{k}_T \cdot \mathbf{r}} \cos \theta_T \\
\frac{1}{\mu_1} (\frac{E_{I,0}}{v_1} e^{i \mathbf{k}_1 \cdot \mathbf{r}} - \frac{E_{R,0}}{v_1} e^{i \mathbf{k}_R \cdot \mathbf{r}}) & = \frac{\hat{k}}{\mu_2 \omega} E_{T,0} e^{i \mathbf{k}_T \cdot \mathbf{r}}
\end{align*}
\]

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For this equality to hold at the boundary $z = 0$ we should have

$$k_I \cdot r = k_R \cdot r = \tilde{k} \cdot r \text{ at } z = 0$$

The $x$ and $y$ components separately must be 0. From this we get:

$$k_{I,x} = k_{R,x} = \tilde{k}_x$$
$$k_I \sin \theta_i = k_R \sin \theta_r = \tilde{k} \sin \theta_T$$

This yields Snell’s relation $\sin \theta_T / \sin \theta_I = n_1/\tilde{n}$ and also $\theta_I = \theta_R$. Simplifying boundary conditions then gives for the **perpendicular** case:

$$E_{I,0} + E_{R,0} = E_{T,0}$$
$$E_{I,0} - E_{R,0} = \frac{\mu_1 \tilde{n}}{\mu_2 \tilde{n}} \cos \theta_T E_{T,0}$$

And for the **parallel** case:

$$E_{I,0} - E_{R,0} = \frac{\mu_1 \tilde{n}}{\mu_2 \tilde{n}} E_{T,0}$$
$$E_{I,0} + E_{R,0} = E_{T,0} \frac{\cos \theta_T}{\cos \theta_I}$$

If we write

$$\tilde{\beta} = \frac{\mu_1 \tilde{n}}{\mu_2 \tilde{n}}$$
$$\alpha = \frac{\cos \theta_T}{\cos \theta_I} = \sqrt{1 - (\frac{\tilde{n}}{n_1})^2 \sin \theta_i}$$

we can write for the **perpendicular** case:

$$E_{T,0}^\perp = \left( \frac{2}{1 + \alpha \beta} \right) E_{I,0}$$
$$E_{R,0}^\perp = \left( \frac{1 - \alpha \beta}{1 + \alpha \beta} \right) E_{I,0}$$

(76)

And for the **parallel** case:

$$E_{T,0}^\parallel = \left( \frac{2}{\alpha + \beta} \right) E_{I,0}$$
$$E_{R,0}^\parallel = \left( \frac{\alpha - \tilde{\beta}}{\alpha + \tilde{\beta}} \right) E_{I,0}$$

(77)

The reflectivity is given by the square of the absolute value of 76,77
Appendix 2 - Derivation of optimal beam waist

Starting from

\[ \frac{d}{dw_0} \left( \frac{1}{2} \left[ 1 + erf\left( \frac{\sqrt{2}d}{w(z_a)} \right) \right] \right) = 0 \]

We can derivate the optimum beam waist as

\[ \frac{d}{dw_0} \left( erf\left( \frac{\sqrt{2}d}{w(z_a)} \right) \right) = 0 \]

\[ \sqrt{2}erf\left( \frac{\sqrt{2}d}{w(z_a)} \right) \frac{d}{dw_0} \left( \frac{1}{w(z_a)} \right) = 0 \]

\[ \frac{d}{dw_0} \left( \frac{1}{w(z_a)} \right) = 0 \]

\[ \frac{1}{w_0^2} + \frac{1}{w_0^2} \frac{z_a \lambda^2}{\pi} \frac{d}{dw_0} \left[ w_0 - \frac{1}{w_0^2} \frac{z_a \lambda^2}{\pi} \right] = 0 \]

\[ w_0 = \frac{z_a \lambda}{\pi} \]

Appendix 3

Figure 21: Beam parameters: focus at \( z = 12.5 \) mm, beam waist \( w_0 = 50 \) µm, \( d = 50 \) µm.
Figure 22: Beam parameters: focus at $z = 12.5 \text{ mm}$, beam waist $w_0 = 50 \mu\text{m}$, $d = 75 \mu\text{m}$.

Figure 23: Beam parameters: focus at $z = 12.5 \text{ mm}$, beam waist $w_0 = 50 \mu\text{m}$, $d = 100 \mu\text{m}$.

Appendix 4

A mathematical way of deriving the phase shift factor in

$$\tilde{\Psi}(s_x, s_y, z) = \tilde{\Psi}(s_x, s_y, z_0) e^{ik(z-z_0)} - i\pi\lambda(s_x^2 + s_y^2)(z-z_0)$$

(78)
is found by looking for the relation between \( \tilde{\Psi}(s_x, s_y, z_0) \) and \( \tilde{\Psi}(s_x, s_y, z) \) from a propagation point of view. The field at a cross-section \( z = z_0 \) can be decomposed as

\[
\Psi(x, y, z_0) = \int \int \tilde{\Psi}(s_x, s_y, z_0) e^{i(2\pi s_x x + 2\pi s_y y)} ds_x ds_y \quad (79)
\]

In addition, \( \Psi \) must still obey the Helmholtz equation (13). In other words:

\[
\frac{\partial^2 \tilde{\Psi}}{\partial z^2} - (2\pi)^2 s_x^2 \tilde{\Psi} - (2\pi)^2 s_y^2 \tilde{\Psi} + \frac{2\pi^2}{\lambda^2} \tilde{\Psi} = 0
\]

\[
\left[ \frac{\partial^2}{\partial z^2} + \left( \frac{2\pi}{\lambda} \right)^2 \left( 1 - \lambda^2 s_x^2 - \lambda^2 s_y^2 \right) \right] \tilde{\Psi} = 0
\]

The solution to this equation is then:

\[
\tilde{\Psi}(x, y, z) = \tilde{\Psi}(x, y, z_0) e^{-ikz \sqrt{1 - \lambda^2 s_x^2 - \lambda^2 s_y^2}}
\]

which by a binomial expansion of the square root can be shown to yield (44).
Populaire samenvatting

Experimenten met ultrakoude gassen, gassen waar de temperatuur enkele microkelvin is, en Bose-Einstein condensaten, gassen die zo koud zijn (nanokelvin) dat zij quantummechanisch gedrag vertonen, behoren tot een relatief recent onderzoeksgebied waarin men interacties tussen atomen kan manipuleren en bestuderen. Een van de mogelijkheden die dit biedt is om een bijdrage te leveren aan het gebied van de quantuminformatie. Om deze koude atomen te manipuleren maakt men gebruik van optische straling, in de vorm van lasers. Lasers produceren coherente straling (dat wil zeggen, alle electromagnetische golven zijn in fase) en kunnen met grote precisie worden ingesteld op een bepaalde frequentie. Door deze frequentie zo te kiezen dat hij het atoom niet aanslaat naar een hogere energiestand, kan voorkomen worden dat het koude gas straling absorbeert, maar tegelijkertijd de atomen wel gepolariseerd raken. Als gevolg van deze polarisatie ondervinden de atomen in het potentiaalveld van de laser een kracht, vergelijkbaar met massa's in een zwaartekrachtpotentiaal, en door deze potentiaal te regelen kan men de atomen dus manipuleren. Zo kan met een enkele laser een dipoolval gebouwd worden, of een optisch rooster met meerdere laserbundels. Om deze ultrakoude gassen te produceren en om ze, zonder warmteuitwisseling met bijvoorbeeld wanden van de vacuumkamer, te conserveren wordt op het Van der Waals-Zeeman Instituut gebruik gemaakt van atoomchips: dit is een kleine chip die in combinatie met spoelen een magnetische val maakt waarin de koude atomen opgesloten zitten in een dunne sigaarvormige wolk op enkele tientallen micrometer van het oppervlak. Door deze kleine afstand en doordat de lasers een relatief grote diameter hebben is het lastig om lasers precies op het gas te mikken, met het gevolg dat een deel van het laserlicht tegen de randen van de chip komt. Als gevolg hiervan treedt diffractie op; diffractie is het buigen van golven wanneer zij een obstakel raken. Bekend voorbeeld van diffractie is bijvoorbeeld het enkelspleet experiment van Young, waarbij vlakke golven die op een smalle spleet vallen een diffractiepatroon produceren op een scherm erachter. Omdat de regelmatige structuur van de optische potentiaal erg belangrijk is (daarom is coherent licht nodig) kan een dergelijk diffractiepatroon dit verstoren. Het is dus van belang om te weten welke invloed diffractie heeft op deze potentiaal. Deze patronen zijn meestal niet analytisch te berekenen, in het bijzonder niet bij ingewikkelde opstellingen, en daarom wordt gebruik gemaakt van de computer om diffractie te simuleren. In de scriptie worden de Fresnel- en Fraunhoferintegralen besproken en gekeken hoe deze hiervoor benut kunnen worden, alsmede hoe deze aangepast kunnen worden om reflecties van de atoomchip in rekening te nemen. Daarnaast wordt een geheel andere techniek, Finite-Difference Time-domain analyse, gebruikt om de Maxwell vergelijkingen (die het gedrag van electromagnetische velden beschrijven) direct op te lossen en deze wordt vergeleken met de Fresnelintegralen.