# Utrecht University 

Debye Institute for Nanomaterials Science
\&
Center for Extreme Matter and Emergent Phenomena
Cold Atom Nanophotonics Group

# Large area photonic crystal cavities: a local density approach 

## Author:

M.C.F. Dobbelaar, BSc.

Supervisors:
S. Greveling, MSc.

Dr. D. van Oosten


#### Abstract

Slowly chirped two-dimensional photonic crystal cavities are promising devices for creating photonic Bose-Einstein condensates. Before experimentally achieving such a condensate, one first has to thoroughly investigate the electromagnetic eigenmodes in such crystals. However, slowly chirped photonic crystals leading to cavities for light will easily have sizes in the order of tens of micrometers. Therefore simulating the behaviour of light in these crystals is very time consuming. In this thesis we demonstrate a novel and intuitive approach to obtain the envelopes of the electromagnetic modes in these crystals. An enormous advantage of this approach is that it can calculate the energies and the envelopes of these eigenmodes to a high accuracy in a few seconds. We model a chirped photonic crystal using a local density approach; we assign a potential energy for light, extracted from photonic bandstructure calculations, to each unit cell of the crystal. We also obtain an effective mass from the curvature of the photonic band at this energy. With these ingredients we are left with the task of solving the corresponding Schrödinger equation, which is an elegant and far less time-consuming exercise than calculating the envelopes of the electromagnetic modes using finite-difference time-domain simulations. In this thesis it is shown that for one- and two-dimensional quadratically chirped photonic crystals the agreement between the envelopes obtained by these simulations and the analytical ones resulting from this model is larger than $90 \%$ for the lowest energy eigenmodes. Moreover, even with small distortions on this quadratic behaviour of the widths of a onedimensional chirped photonic crystal, the corresponding numerically obtained solutions of the Schrödinger equation clearly have an excellent agreement with the simulated mode envelopes.


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## 1 Introduction

Ninety years ago, Satyendra Bose developed the foundations of the statistical mechanics of an ideal photon gas [1]. Albert Einstein generalized his ideas to bosonic matter [2]. In the latter case, bosons in a condensed state that we now call a Bose-Einstein condensate (BEC) are described. In this quantum phase a macroscopic amount of particles occupies the quantum ground state. Much later, theoretical methods were developped to be able to achieve photonic BECs by introducing thermalization mechanisms of the photons that do not involve a decrease of the photon density (see for instance Zel'Dovich et al. [3]).
Fifteen years after the first experimental realization of an atomic BEC in 1995 [4, 5], the Quantum Optics Group of the University of Bonn led by Martin Weitz achieved the first experimentally realized photonic BEC [6]. There, the photons were confined in two dimensions using an optical cavity and brought into thermal equilibrium by continuous absorption and emission by a dye solution. The curved mirrors of the cavity also introduce a cut-off frequency in the dispersion relation in the transverse direction, thereby giving the photons an effective mass. This BEC can thus also be seen as a condensate of massive bosons, as in the case of an atomic BEC.
In our Cold Atom Nanophotonics group we plan to realize such a condensate in a different way, namely by using a chirped photonic crystal ( $\mathrm{PhC} \mathrm{)} \mathrm{of} \mathrm{semiconductor} \mathrm{material}$. PhC will give rise to a harmonic trapping potential. The semiconductor material takes care of the thermalization of the photons. A large advantage of this approach is that by tuning the PhC parameters, the periodic character of the structure can be more or less pronounced and a large nonlinearity can be obtained. This gives the opportunity to look at quantum phase transitions from a BEC to an insulating state whereby there is a small integer number of photons located in each unit cell of the crystal. This would be the first experimental achievement of such a phase transition of light.
With these exciting goals in mind, we first need to investigate the electromagnetic eigenmodes of such a PhC.
Besides being of fundamental interest, these PhCs have many applications such as omnidirectional mirrors [7], heterostructure cavities [8], slow-light generation [9], PhC LEDs [10], solar cells [11] and (chirped [12]) PhC fibers [13].
For all these applications, the design of the crystal effects the light behaviour rigorously. This behaviour usually is simulated during the development of the PhC . This requires large computational power and a lot of computing time. These simulations are normally done using finite-difference time-domain calculations, which break up time and space in very tiny pieces and compute the solutions to the Maxwell equations numerically at each grid point for each time step.
In this thesis a novel model is described to obtain the envelopes of these modes in one- and two-dimensional non-absorbing PhCs in a few seconds. It involves a local density approach which gives rise to an effective potential. We also assign the photons in the crystal an effective mass so that we are left with solving a simple Schrödinger equation to find the envelopes of the modes in the PhC. Because of the low computational effort, this model opens up new possibilities to develop and understand large devices relevant to optoelectronics, photovoltaics and solid-state lighting. An article based on this thesis will be submitted to the open-access optics journal Optics Express [14].

## 2 Theory

In this chapter the basic theoretical concepts of one and two-dimensional PhCs are introduced. Afterwards a novel and intuitive model is introduced for chirped PhCs. Central in this model is a local density approximation, in which an effective potential energy and effective mass are assigned to photons in the crystal. Hereby, the problem of finding the electromagnetic eigenmodes in the crystal is mapped to solving the much simpler Schrödinger equation. In this way the envelopes of these eigenmodes can be calculated very quickly, circumventing time-consuming computer simulations.

### 2.1 Introduction to photonic crystals

The subject of PhCs is a fascinating interplay between solid state physics and electromagnetism. A lot of concepts and terminology that are used in the field of solid state physics to describe the behaviour of electrons in crystals are transferred to the field of PhCs. Here we can talk about optical or photonic bandstructures and bandgaps when describing the dispersion relation of the light in a PhC . On the other hand, since one knows that light can be considered as an electromagnetic wave, classical electromagnetism comes into play.
We will assume that the reader is familiar with the basics of both electromagnetism and solid state physics. The main reference for this section is Joannopoulos et al. [15].

### 2.1.1 Electromagnetism

As a natural starting point we begin with stating the four well known laws of classical electromagnetism, the Maxwell equations [16]

$$
\begin{array}{ll}
\nabla \cdot \mathbf{D}=\rho_{f}, & \nabla \times \mathbf{E}=-\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \cdot \mathbf{B}=0, & \nabla \times \mathbf{H}=\mathbf{J}_{f}+\frac{\partial \mathbf{D}}{\partial t} \tag{2.1}
\end{array}
$$

where $\mathbf{E}, \mathbf{D}$ and $\mathbf{B}$ denote the electric field, the electric displacement and the magnetic field, respectively. $\mathbf{H}=\mu_{0}^{-1} \mathbf{B}-\mathbf{M}$, where $\mu_{0}=4 \pi \times 10^{-7} \mathrm{~N} / \mathrm{A}^{2}$ denotes the permeability of free space and $\mathbf{M}$ the magnetization. $\rho_{f}$ and $\mathbf{J}_{f}$ indicate the free charge and free current densities. These general equations are valid in all macroscopic matter, but we will confine our interest to the subclass of dielectric materials where, to a good approximation, there are no free charges nor currents. If the fields under consideration are not too strong, the higher order susceptibilities that relate the polarizability to applied electric fields can be disregarded. The medium will be assumed to be isotropic as well. Since we shall only use fixed relative permitivities of 1 (air) and 12 in our simulations, the possible dispersion of the (relative) dielectric constant $\varepsilon$ is neglected. It is also a plausibel assumption that we are in a non-absorbing regime, so that $\varepsilon \in \mathbb{R}_{>0}$. Finally, in most cases of interest regarding PhCs the relative permeability is extremely close to unity, i.e. $\mu=1$.

All these assumptions result in the following equations, which the reader can readily verify

$$
\begin{align*}
\nabla \cdot \mathbf{H} & =0, \\
\nabla \cdot(\varepsilon \mathbf{E}) & =0, \tag{2.2}
\end{align*} \quad \nabla \times \mathbf{E}=-\mu_{0} \frac{\partial \mathbf{H}}{\partial t}, ~=\varepsilon_{0} \varepsilon \frac{\partial \mathbf{E}}{\partial t}, ~ l
$$

where $\varepsilon_{0}=8.854187817 \times 10^{-12} \mathrm{C}^{2} / \mathrm{Nm}^{2}$ denotes the permittivity of free space, all fields depend on position and time, and the dielectric function $\varepsilon$ only on the position $\mathbf{r}$.
We can use separation of variables to separate the time-dependent part from the spatial dependence and we can write the resulting harmonic modes as

$$
\begin{equation*}
\mathbf{H}(\mathbf{r}, t)=\mathbf{H}(\mathbf{r}) \mathrm{e}^{-i \omega t} \quad \text { and } \quad \mathbf{E}(\mathbf{r}, t)=\mathbf{E}(\mathbf{r}) \mathrm{e}^{-i \omega t} . \tag{2.3}
\end{equation*}
$$

Here, $\omega$ denotes the angular frequency of such an electromagnetic mode. Substituting these expressions into Equations 2.2 results in two sets of equations for the spatial parts. The first one consists of the divergence equations, which imply that the electromagnetic field modes are built up out of transverse plane waves. The other two are of more interest and can be written as

$$
\begin{equation*}
\nabla \times \mathbf{E}=i \omega \mu_{0} \mathbf{H} \tag{2.4}
\end{equation*}
$$

and

$$
\begin{equation*}
\nabla \times \mathbf{H}=-i \omega \varepsilon_{0} \varepsilon \mathbf{E} \tag{2.5}
\end{equation*}
$$

Eliminating the electric field from the above equations and using $c^{-2}=\varepsilon_{0} \mu_{0}$ we arrive at the wave equation

$$
\begin{equation*}
\hat{\Theta} \mathbf{H}:=\nabla \times\left(\varepsilon^{-1} \nabla \times \mathbf{H}\right)=\left(\frac{\omega}{c}\right)^{2} \mathbf{H}, \tag{2.6}
\end{equation*}
$$

where we also have defined the Hermitian operator $\hat{\Theta} .{ }^{1}$ Because of the hermiticity of the operator $\hat{\Theta}$, we know that the eigenvalues $\left(\frac{\omega}{c}\right)^{2}$ are real and that eigenmodes with different eigenvalues are orthogonal to each other. Furthermore, the assumption that $\varepsilon>0$ implies that $\omega$ is real. The wave equation can in general only be solved using numerical methods. These methods try to use as many symmetry arguments as possible. This is a general feature in modern physics and the importance of symmetry can hardly be overrated. We shall treat it in the context of PhCs in the next subsection.

### 2.1.2 Symmetry

When a system posseses a certain symmetry $\mathcal{S}, \hat{\Theta}$ commutes with the associated symmetry operator $\hat{\mathcal{S}}$. This means that this symmetry operator and the more intricate operator $\hat{\Theta}$ have a complete set of eigenfunctions in common. Using this, one can classify these eigenfunctions and gain insight in the allowed electromagnetic modes.
Let us now consider a one-dimensional PhC with a discrete translational symmetry of the dielectric function $\varepsilon(\mathbf{r})$ in the $x$-direction and continuous translational symmetry in the perpendicular directions, so that $\varepsilon(\mathbf{r})=\varepsilon(\mathbf{r}+\boldsymbol{a})$ for all $\mathbf{r} \in \mathbb{R}^{3}$, where $\boldsymbol{a}$ denotes the lattice vector. Eigenfunctions of $\hat{T}_{x}^{d}$, the translational operator over a distance $d$, are plane waves $e^{i k_{x} x}$, as in the case of continuous translational symmetry

$$
\begin{equation*}
\hat{T}_{x}^{d} e^{i k_{x} x}=e^{i k_{x}(x-d)}=e^{-i k_{x} d} e^{i k_{x} x} \tag{2.7}
\end{equation*}
$$

${ }^{1}$ With the inner product between two fields $\mathbf{F}_{\mathbf{1}}$ and $\mathbf{F}_{\mathbf{2}}$ defined by $\left\langle\mathbf{F}_{\mathbf{1}}, \mathbf{F}_{\mathbf{2}}\right\rangle=\int \mathbf{F}_{\mathbf{1}}{ }^{*} \mathbf{F}_{\mathbf{2}}$ d $\mathbf{r}$, see Joannopoulos et al. [15] for a proof of the hermiticity.
so that we see that the corresponding eigenvalue is $e^{-i k_{x} d}$. In contrary to the continuous/homogeneous case, we now have a degeneracy in momentum space, since adding an integer number times $\frac{2 \pi}{a}$ to some $k_{x}$ yields the same eigenvalue. As the wave equation is a linear differential equation, a linear combination of degenerate eigenfunctions or eigenmodes gives another eigenmode. We can thus write such a mode as

$$
\begin{equation*}
\mathbf{H}_{\mathbf{k}}(\mathbf{r})=e^{i k_{\perp} \cdot \rho} \sum_{m} c_{k_{x}} e^{i\left(k_{x}+m a^{*}\right) x}=e^{i \mathbf{k} \cdot \mathbf{r}} \sum_{m} c_{k_{x}} e^{i m a^{*} x}=e^{i \mathbf{k} \cdot \mathbf{r}} u_{k_{x}}(x) \tag{2.8}
\end{equation*}
$$

where $\mathbf{k}=\left(k_{x}, k_{y}, k_{z}\right), \rho=(y, z)$ denotes the cartesian coordinate in the perpendicular plane, and $a^{*}=\frac{2 \pi}{a}$ the primitive reciprocal lattice vector. The function $u_{k_{x}}(x)$ is thus a periodic function with the periodicity of the crystal. We conclude that we can write an eigenmode as a planewave modulated by such a periodic function, i.e. in Bloch's form.
The periodicity in momentum space allows us to restrict ourselves to consider only wavevectors $\mathbf{k}$ with $k_{x} \in\left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$, which is called the first Brillouin zone (BZ), analogous to the solid state physics terminology.
The above discussion generalizes straightforwardly to two and three dimensions. In the latter case the eigenmodes can be written as

$$
\begin{equation*}
\mathbf{H}_{\mathbf{k}}(\mathbf{r})=e^{i \mathbf{k} \cdot \mathbf{r}} u_{\mathbf{k}}(\mathbf{r}), \tag{2.9}
\end{equation*}
$$

where $u_{\mathbf{k}}(\mathbf{r})$ again obeys the periodicity of the crystal, and $\mathbf{k}$ can be chosen in the first BZ. In the case of a two-dimensional PhC with discrete translational periodicity in the $x$ and $y$ directions and continuous translational periodicity in the $z$ direction, there is also a mirror symmetry $\mathcal{M}_{z}$ with $\mathcal{M}_{z}(x, y, z)=(x, y,-z)$ that leaves the structure invariant. This leads to a classification in terms of polarization of the eigenmodes of such a PhC that divides them in even (unchanged under mirroring) and odd (sign change under mirroring) modes. As electric fields transform as vectors under reflections and magnetic fields as pseudovectors, we see that the even modes can only have electric components in the ( $x, y$ )-plane and a magnetic component in the $z$-direction. Vice versa for the odd modes. The former are in the field of PhCs called transverse-electric (TE) modes, whereas the latter are referred to as transverse-magnetic (TM) modes.
An interesting consequence of symmetry is the time-reversal invariance. By complex conjugating (or changing the sign of time in Equation 2.3) the wave equation and noting that $\mathbf{H}_{\mathbf{k}}^{*}$ equals $\mathbf{H}_{-\mathbf{k}}$ (use Equation 2.9), we infer that $\mathbf{H}_{-\mathbf{k}}$ and $\mathbf{H}_{\mathbf{k}}$ have the same eigenvalues and thus frequencies. The optical band structures of materials that satisfy the assumptions made earlier thus have inversion symmetry.

### 2.1.3 One-dimensional photonic crystals

We now investigate the case of one-dimensional PhCs in a bit more detail. These crystals generally consist of slabs of dielectric material that extend to infinity in two perpendicular ( $x$ and $y$ ) directions. In the remaining $(z)$ direction the constituting slabs are organized in a periodic manner. As in the previous subsection, we call the accompanying lattice vector $\boldsymbol{a}$. As an easy, fundamental and interesting case let us now look at a one-dimensional PhC consisting of two alternatingly stacked dielectric materials with dielectric constants $\varepsilon_{1}$ and $\varepsilon_{2}$. As we know, the $z$ direction is of most interest, so we shall confine ourselves to wavevectors parallel to $k_{z}$. Because of the periodicity we can further restrict our attention to the wavevectors in the first BZ. Finally, as discussed in Subsection 2.1.2, the dispersion relation obeys inversion
symmetry so that we only have to look at non-negative values of $k_{z}$. This region is called the irreducible BZ.
Now, if $\varepsilon_{1}=\varepsilon_{2}$, the material actually is homogeneous. Putting plane wave solutions $\mathbf{H}_{0} e^{i k_{z} z}$ into the wave equation yields the familiar equation for the light line: $\omega=c k_{z} / \sqrt{\varepsilon}$. This is a straight line in the dispersion diagram ${ }^{2}$. If we let $\varepsilon_{2}$ increase a bit and assign it a relative slabwidth of 0.45 of the lattice constant $a=|\boldsymbol{a}|$, then the line is perturbed and a first photonic band gap arises at the edge of the first BZ as can be seen in Figure 2.1. This bandstructure was computed using the open source MIT Photonic Band package. ${ }^{3}$ In that region of frequencies


Figure 2.1: Optical bandstructure (blue) of a one-dimensional PhC with a dielectric slab width $w=0.45$. In red a local parabolic approximation, which we will use later on to assign an effective mass to photons in this PhC (see Equation 2.13), is depicted. The vertical gray dashed line indicates the edge of the first BZ.
there is no single wavevector that can sustain an eigenmode of the crystal. There are at least two ways to qualitatively account for this gap. We can first use an argument often employed in solids state physics and look at a plane wave falling onto the crystal in the $z$ direction. This wave partially reflect at each dielectric interface. These reflections interfere constructively if the wavelength $\lambda$ of the incoming wave is exactly $2 a$. This occurs when $k= \pm \frac{\pi}{a}$, which are the outer edges of the first $\mathrm{BZ}^{4}$. Another argument uses symmetry considerations and the fact that it is energetically favourable for a mode to have the energy of its electric field component located at regions of high dielectric constant ${ }^{5}$ In this case, we look at the modes just beneath and above the bandgap. As we just recalled, their wavelength is $2 a$. Since we have a mirror symmetry in the plane lying in the center of the central slab with the higher dielectric constant

[^0]$\varepsilon_{2}$, the modes thus have to be even or odd with respect to this symmetry. Obviously, the even one has the highest intensity of its electric field in regions with a high dielectric constant and vice versa for the odd mode. We can thus understand that the former one has a lower frequency than the latter one. Also, we can argue that this effect is more pronounced if the difference $\left|\varepsilon_{1}-\varepsilon_{2}\right|$ increases. The lower and upper band are also referred to as the dielectric and air band, respectively.

### 2.1.4 Two-dimensional photonic crystals

Two-dimensional PhCs have a dielectric function $\varepsilon$ that obeys $\varepsilon(\mathbf{r})=\varepsilon(\mathbf{r}+\boldsymbol{b})$ for vectors $\mathbf{r} \in \mathbb{R}^{3}$ and for $\boldsymbol{b}$ in the two-dimensional lattice. Typically one should think of a regularly spaced set of rods of a certain material embedded in some other medium. In contrast to the one-dimensional case, we encounter a new feature that is not present in the classical field of solid state physics. Namely, polarization starts to play a prominent role, e.g. in the dispersion diagrams. As discussed in Subsection 2.1.2, modes can be divided into two classes when considering twodimensional PhCs: TM and TE modes. This means the band structures will also be subdivided into these two components. One thus expects large bandgaps between consecutive bands when the difference in degree of localization at high $\varepsilon$ regions is large between the modes represented by these bands. Since the TM modes have their electric field pointing parallel to all dielectric interfaces in the PhC , they can be concentrated in merely the high $\varepsilon$ material, whereas the TE modes have to cross the dielectric boundaries (considering a PhC consisting of dielectric rods surrounded by air) and have to have large portions of their modes residing in the low $\varepsilon$ medium as well. This explains why the bands of TE and TM modes can be very different from one another. In a PhC containing such rods, we thus expect that the energy difference between successive TE bands are smaller than between TM bands (keeping in mind that the upper band has to be perpendicular to the lower band).
The situation is different in a PhC that does not consist of disconnected dielectric rods, but for instance equals the union of a one-dimensional PhC with thin dielectric slabs positioned parallel to the ( $\mathrm{x}, \mathrm{z}$ )-plane and an identical one with slabs parallel to the ( $\mathrm{y}, \mathrm{z}$ )-plane. In this way they together form a network of squares of dielectric material, as seen in the (x,y)-plane. Now, the lowest frequency electric field in the $(x, y)$-plane can be concentrated in these dielectric planes and the next one, being orthogonal to the first one, has to have a much lower concentration in these planes. This can give rise to a gap between the TE bands.
Combining the insights from the discussion above, we now want to design a structure that exhibits a complete photonic bandgap. Then, for certain frequencies, the PhC will act as a mirror for incoming waves of any polarization. This structure incorporates elements of both PhCs given above, in that it consists of rods and the dielectric medium is also one globally connected piece of material. The rods, now really air holes, are placed in a triangular lattice. In this way a good compromise can be made between isolated high $\varepsilon$ regions (favours large TM bandgaps) and connected high $\varepsilon$ regions (favours large TE bandgaps). Namely, by making these holes large enough with respect to the size of unit cell, the dielectric material that remains is so small that, in a $z$ slice, it consists of small areas connected by thin bridges between them. In this way, both the EM and TM modes simultaneously exhibit photonic bandgaps as can be seen in Figure 2.2.
The construction of the $1^{\text {st }} \mathrm{BZ}$ for this triangular lattice is the same as in the case for electrons in crystals. In general, first the primitive or basis reciprocal lattice vectors $b^{i}$ have to be determined from the basis lattice vectors $b_{i}$. For that we construct the matrix $B_{\text {rec }}$ as composed of $\left\{b^{i}\right\}_{i}$ as columns and similarly the matrix $B$ as composed of $\left\{b_{i}\right\}_{i}$ as columns, both using


Figure 2.2: Optical bandstructure with the TE (red) and TM (green) bands of a two-dimensional PhC consisting of a triangular lattice of air holes, embedded in a dielectric medium with dielectric constant $\varepsilon=12$. The radius of these holes equals $\rho=0.42$. The blue horizontal region represents the complete photonic bandgap.
the natural ordening of the index. We can then write their relation as $B_{\text {rec }}=2 \pi\left(B^{T}\right)^{-1}$, where a $T$ indicates the transpose of a matrix ${ }^{6}$.
In the case of a two-dimensional triangular lattice, we can take the first two basis vectors $b_{1}, b_{2}$ to be the two vectors pointing from one air hole to two of its neighboring air holes $a\left(\frac{1}{2}, \pm \frac{\sqrt{3}}{2}, 0\right)$, where $a$ equals the distance between two adjacent air hole centers. For the third basis vector $b_{3}$ we conveniently choose $(0,0,1)$. Performing the matrix operations indicated above we arrive at the following expressions for the basis reciprocal lattice vectors: $b^{1}, b^{2}=\frac{2 \pi}{a}\left(1, \pm \frac{1}{\sqrt{3}}, 0\right)$ and $b^{3}=(0,0,2 \pi)$.
Now, a BZ is constructed in such a manner that there is a unique wavevector $\mathbf{k}$ in this region that corresponds to the wavevector of a given Bloch function. The $1^{\text {st }} \mathrm{BZ}$ is such a region containing $\mathbf{k}=0$ and it is defined in the following way. For each basis reciprocal lattice vector and their opposite (negative) vectors a plane can be considered that intersect this vector halfway and perpendicular, so that its normal points in the direction of this reciprocal vector. The volume bounded by these planes equals the $1^{\text {st }} \mathrm{BZ}$ [17]. It is thus the set of $\mathbf{k}$-points that have a distance to $\mathbf{k}=0$ that is not larger than the distance to any other reciprocal lattice vector ${ }^{7}$. If also non-translational symmetries of the crystal are taken into account, we can further narrow our attention down to the irreducible BZ as indicated in gray in the inset of Figure 2.2. A triangular or hexagonal lattice thus yields a hexagonal reciprocal lattice (which is rotated over $\frac{\pi}{6}$ radians with respect to the original one). The resulting $1^{\text {st }} \mathrm{BZ}$ can be seen as unrotated with respect to the original lattice. The vertices of the irreducible BZ carry the

[^1]same names as in solid state physics and are also indicated in the same figure.

### 2.1.5 The notion of effective mass

The air band (which in Figure 2.2 is the $3^{\text {rd }}$ TM band) can of course be approximated around its minimum $\mathbf{k}_{\text {min }}$ by a $2^{\text {nd }}$ order Taylor expansion in $\mathbf{k}$, where the linear term vanishes

$$
\begin{equation*}
E(\mathbf{k})=E\left(\mathbf{k}_{\min }\right)+\frac{1}{2!}\left(\mathbf{k}-\mathbf{k}_{\min }\right)^{T} \mathrm{D}^{2} E\left(\mathbf{k}_{\min }\right)\left(\mathbf{k}-\mathbf{k}_{\min }\right) . \tag{2.10}
\end{equation*}
$$

Here, $\mathrm{D}^{2} E\left(\mathbf{k}_{\text {min }}\right)$ denotes the Hessian ${ }^{8}$ of the energy of this band at $\mathbf{k}_{\text {min }}$. One thus immediately sees that the group velocity $\mathrm{D} \omega(\mathbf{k})$ of a mode residing in the air band at such a minimum equals zero ${ }^{9}$.
The curvature of any dispersion gives rise to the notion of an effective mass of the particle under consideration. This relation is well-known in solid state physics where the particle in question is a valence electron in some periodic potential generated by the nuclei and lower-shell electrons [18]. In general, the dispersion can be anistropic. In that general case the effective mass $m^{*}$ is defined by

$$
\begin{equation*}
\left(\frac{1}{m^{*}}\right)_{i, j}=\hbar^{-2} \frac{\partial^{2} E}{\partial \mathbf{k}_{i} \partial \mathbf{k}_{j}} \tag{2.11}
\end{equation*}
$$

Qualitatively we can thus say that a large curvature corresponds to a small effective mass. In the isotropic case the Hessian reduces to a scalar multiple of the identity matrix and the effective mass then can be simply defined by

$$
\begin{equation*}
m^{*}=\hbar^{2}\left(\frac{\partial^{2} E}{\partial \mathbf{k}^{2}}\right)^{-1} \tag{2.12}
\end{equation*}
$$

Combing this expression with Equation 2.10, the dispersion near the minimum can be expressed as

$$
\begin{equation*}
E(\mathbf{k})=E\left(\mathbf{k}_{\min }\right)+\frac{\hbar^{2}}{2 m^{*}}\left(\mathbf{k}-\mathbf{k}_{\min }\right)^{2} \tag{2.13}
\end{equation*}
$$

which thus (approximately) holds when the dispersion around $\mathbf{k}_{\text {min }}$ is (nearly) isotropic.

### 2.2 Chirped photonic crystals

An important variation on the notion of a PhC is a chirped PhC , for which a parameter like the local mean dielectric constant $\varepsilon$ is slowly varied in space, but locally has the structure of a PhC. A chirped PhC itself thus cannot be classified as a (by definition periodic) PhC, however if the chirping rate is slow enough the (almost) periodic nature still gives us the opportunity to talk about unit cells, bandstructures, etc. In fact, we will later show that under this condition, these notions are very useful and should also be considered as slowly varying inside the crystal.

[^2]
### 2.2.1 Cavities

As alluded to in Chapter 1, the goal is to create a cavity and, at the same time, a periodic potential for photons. For that, we want to use two-dimensional triangular chirped PhCs of air rods in a dielectric medium, where the dielectric material has a dielectric constant of 12 . As shown in Subsection 2.1.4, a complete bandgap appears when the radius of the cylindrical air rods is large enough. For photons with an energy just above the bandgap, the bottom energy $E_{k_{\min }}$ can be interpreted as its potential energy. In a chirped PhC we can now use the idea mentioned above and thus locally define a potential that one would assign to it when it was part of a periodic PhC (local density approximation). Increasing the hole size means that the bottom of the air band, i.e. the effective potential, shifts to higher energies. A cavity can thus be created by making the hole size larger while going further away from the center of the crystal. This trapping effect is for instance also used in double-heterostructure cavities [19]. By slowly chirping one can thus create a cavity in which light can be trapped but also experiences a practically periodic potential. Electromagnetic field modes can thus be expected to be written (within a good approximation) as a periodic part, modulated by a slowly varying envelope, as suggested by Vigneron et al. [20]. Using Equation 2.9, the magnetic field of the modes can thus be written as

$$
\begin{equation*}
\mathbf{H}(\mathbf{r})=\psi(\mathbf{r}) \sum_{\left\{\mathbf{k}_{\min }\right\}} \mathcal{H}_{\mathbf{k}_{\min }}(\mathbf{r}) e^{i \mathbf{k}_{\min } \cdot \mathbf{r}}, \tag{2.14}
\end{equation*}
$$

where the sum runs over the wavevectors in the $1^{\text {st }} \mathrm{BZ}$ where the air band attains its minimum. The scalar function $\psi(\mathbf{r})$ denotes the envelope. For the electric part a similar equation holds. It is this envelope function $\psi(\mathbf{r})$ that we want to know for a given chirped PhC . This function only arises because of the chirping of the crystal and does not contain information on the periodicity nor the local structure of the PhC . A light mode populating the air band ${ }^{10}$ experiences an effective potential that we can easily calculate. We can also assign a mass to it; the effective mass $m^{*}$ that we derive from the curvature at the minimum of the air band. For a certain range of hole sizes and thus bandstructures, it turns out (as we shall later show) that this effective mass can, to a good approximation, be considered constant.
We thus encounter a particle (the photon) that has a mass $m^{*}$ and experiences an effective potential $V(\mathbf{r})$. It thus satisfies the wave equation for such particles ${ }^{11}$

$$
\begin{equation*}
\left(-\frac{\hbar^{2}}{2 m^{*}} \nabla^{2}+V(\mathbf{r})\right) \phi(\mathbf{r})=E \phi(\mathbf{r}) \tag{2.15}
\end{equation*}
$$

which is of course the time-independent Schrödinger equation. In this equation the eigenvalue $E$ denotes the energy of the particle which state is represented by the wavefunction $\phi(\mathbf{r})$. Note that we used the letter $\psi$ to denote the envelope function of the electromagnetic mode and the letter $\phi$ for the corresponding wavefunction because these are exactly the functions we want to compare quantitatively.
Or more specifically, we want to investigate how well the wavefunction that we obtain by solving the Schrödinger equation using only the effective mass and potential (employing bandstructure calculations) matches the envelope function of the mode, which is computed by simulations that numerically solve Equation $2.6^{12}$.

[^3]To extract the envelope function $\psi$ from the simulations, we assume that the simulated mode has the form given by Equation 2.14. Furthermore, if the crystal is chirped slowly enough, the mode is delocalized over a large enough area so that its (spatial) Fourier transform (FT) consists of small (and thus isolated) islands in momentum space, i.e. the width of the FT of $\psi(\mathbf{r})$ is much smaller than the distance between the vectors $\mathbf{k}_{\text {min }}$. The FT of the product of two functions results in the convolution of the FTs of the two functions. The FT of equation 2.14 can thus be written as

$$
\begin{equation*}
\tilde{\mathbf{H}}(\mathbf{k})=\tilde{\psi}(\mathbf{k}) * \tilde{\mathcal{H}}_{\mathbf{k}_{\text {min }}}(\mathbf{k}) \tag{2.16}
\end{equation*}
$$

where $*$ denotes a convolution and we have defined $\tilde{\mathcal{H}}_{\mathbf{k}_{\text {min }}}(\mathbf{k})$ as

$$
\begin{equation*}
\sum_{\left\{\mathbf{k}_{\min }, \kappa\right\}} \tilde{\mathcal{H}}_{\mathbf{k}_{\min }, \kappa} \delta\left(\mathbf{k}-\left(\mathbf{k}_{\min }+\kappa\right)\right) \tag{2.17}
\end{equation*}
$$

where $\kappa$ runs over the reciprocal lattice vectors (because of the periodicity of the $\mathcal{H}_{\mathbf{k}_{\text {min }}}(\mathbf{r})$ term in Equation 2.14).
In momentum space we subsequently select one isolated peak centered at a $\mathbf{k}_{\text {min }}$ in the $1^{\text {st }} \mathrm{BZ}$ by putting a mask ${ }^{13}$ around it. Hence we are left with the following expression

$$
\begin{equation*}
\tilde{\psi}(\mathbf{k}) * \tilde{\mathcal{H}}_{\mathbf{k}_{\min }} \delta\left(\mathbf{k}-\mathbf{k}_{\min }\right) \tag{2.18}
\end{equation*}
$$

Taking the inverse FT hereof, multiplying with $e^{-i \mathbf{k}_{\min } \cdot \mathbf{r}}$ and normalizing, yields the envelope $\psi(\mathbf{r})$.
We shall employ this recipe in both one and two-dimensional chirped PhCs in order to compare this envelope with the solutions of the corresponding Schrödinger equation.

[^4]
## 3 Results

In this chapter we discuss the FDTD simulation results and investigate how well our model works in three different cases. Firstly, we consider a one-dimensional quadratically chirped PhC . Secondly, we continue with a one-dimensional crystal on which noise in the slab width has been introduced. Lastly, we examine a two-dimensional triangular PhC that is chirped quadratically.

### 3.1 One-dimensional cavity

In this section we investigate our model for a perfect one-dimensional harmonic cavity and for a distorted one-dimensional harmonic cavity. In the first case we can use the analytical eigenstates of the quantum harmonic oscillator to quantify our local density approach. In the second case we need to use a numerical tool to solve the Schrödinger equation.

### 3.1.1 Effective mass and effective potential

The one-dimensional chirped PhC investigated here, contains dielectric slabs with a dielectric constant of $\varepsilon=12$. The normal of the slabs point parallel to the $x$-direction. We again denote the slab width $w$ as a fraction of the lattice constant $a(=500 \mathrm{~nm})$. For a whole range of widths we have calculated the (optical) bandstructure. From these bandstructures we obtained $E_{\min }(w)$, the energy at the minimum of the air band, which depends on the slab width $w$. This relation is plotted at the top of Figure 3.1. Beneath it the effective mass $m^{*}$, calculated from the curvature at the same wavevector $\mathbf{k}_{\min }$ (as explained in Subsection 2.1.5), is depicted as a function of the width.
One immediately sees that if we confine ourselves to the widths ranging from 0.35 until 0.45 , we can take the effective mass to be constant to a good approximation. We can also fit a line to the energy curve in this range. In this way, we arrive at the linear empirical relation between $E_{\min }$ and $w$

$$
\begin{equation*}
E_{\min }(w)=-1.49 w+1.38 \tag{3.1}
\end{equation*}
$$

where $E_{\text {min }}$ is given in units of electronvolt (eV).
As we would like to create a harmonic potential for the photons in the cavity, we thus have to decrease the width quadratically away from the center:

$$
\begin{equation*}
w(x)=w_{\max }-\left(\frac{x}{\eta}\right)^{2} \tag{3.2}
\end{equation*}
$$

where $w_{\max }$ denotes the center width, $x$ the distance from the center of the PhC and $\eta$ is a parameter that controls the chirping rate. The larger $\eta$ is, the slower the width decreases away from the crystal center and the larger the entire crystal becomes.

### 3.1.2 FDTD results

As we now have designed a chirped PhC, we want to find the electromagnetic modes that are sustained in this crystal with an energy just above the first (optical) bandgap. We calculate


Figure 3.1: Bandstructure calculations for a range of slab widths $w$. In (a) the energy of the bottom of the band $E_{\min }(w)$ (red circles) is depicted. A first order polynomial (blue) is fitted to the data points that lie within the range depicted by the two vertical black dashed lines. In (b) the effective mass $m^{*}$ is indicated by green triangles.
these modes by performing FDTD simulations using the software package Meep ${ }^{14}$. For these simulations we place a point current source $H_{z}$ in the neighborhood of the center, away from any symmetry point. At this excitation point we create a broad electromagnetic pulse with a center frequency $f_{\text {cen }}$ close to the frequency that corresponds to the bottom of the air band. The pulse width $f_{\Delta}$ is relatively broad, as we want to cover a range of frequencies to excite and detect also higher modes so that we can compare these modes with the corresponding higher harmonics of a harmonic potential. Letting the pulse evolve over some time, the FDTD simulation yields a combination of the modes that were excited and lists their eigenfrequencies. As we are interested in the separate mode profiles, we subsequently use narrow pulses, with a width denoted by $f_{\delta}$, centered at these frequencies and run a new simulation to get clear mode patterns, i.e. the field distribution for the modes. The number of the modes we find depends on the width of the broad excitation pulse.
The spatial resolution of a one-dimensional simulation is given by the number of pixels that are used per unit cell. If one increases this spatial resolution, the program automatically decreases

[^5]the time steps accordingly. This means, for instance, for a two-dimensional simulation that a doubling of the resolution amounts to approximately an eight fold increase in computation time. It turns out that for the parameters listed in Table 3.1, that from a resolution of 32 on, the mode profile changes are very minimal ${ }^{15}$.
The units that are employed in the table match the units used by the MIT software ${ }^{16}$.

| Parameter | Value |
| :--- | ---: |
| $a$ | 500 nm |
| $\eta$ | $40 a$ |
| $w_{\max }$ | 0.45 |
| resolution | $128 \frac{\mathrm{px}}{a}$ |
| $f_{\Delta}$ | $0.2 \frac{c}{a}$ |
| $f_{\text {cen }}$ | $0.3 \frac{c}{a}$ |
| $f_{\delta}$ | $0.001 \frac{c}{a}$ |
| excitation point | $-4 a$ |

Table 3.1: Parameters used for the simulation of light modes in a one-dimensional chirped PhC , where $c$ denotes the speed of light in vacuum.

An FDTD simulation using the values of Table 3.1 results in the mode patterns of Figure 3.2. Here the square of the absolute value of the modes are plotted in blue, together with the dielectric function $\varepsilon(x)$ of the PhC in gray.

### 3.1.3 Local density results

To test our model we want to compare the envelopes of these modes with the lowest-energy wavefunctions of the corresponding one-dimensional quantum harmonic oscillator. The curvature of the harmonic potential (arising from Equations 3.1 and 3.2) determines the spatial extent of the wavefunctions. This extent can be neatly expressed by its harmonic oscillator length $l_{\mathrm{HO}}=\sqrt{\frac{\hbar}{m^{*} \Omega}}$, where $\Omega$ denotes the (constant) frequency spacing between the wavefunctions. If we define $\xi$ as the dimensionless variable $\frac{x}{l_{\mathrm{HO}}}$, we can write the well-known analytical solutions of the Schrödinger equation for a particle with mass $m^{*}$ trapped in the one-dimensional harmonic potential $\frac{\hbar}{2} \Omega \xi^{2}$ as [21]

$$
\begin{equation*}
\phi_{n}(\xi)=\left(\sqrt{\pi} l_{\mathrm{HO}}\right)^{-\frac{1}{2}} \frac{1}{\sqrt{2^{n} n!}} H_{n}(\xi) e^{-\xi^{2} / 2} \tag{3.3}
\end{equation*}
$$

where $n \in \mathbb{N}_{0}$ and $H_{n}(\xi)$ denotes the $n^{\text {th }}$ Hermite polynomial. Their respective energies are given by

$$
\begin{equation*}
E_{n}=\left(\frac{1}{2}+n\right) \hbar \Omega \tag{3.4}
\end{equation*}
$$

In Figure 3.2 we depict the squared absolute values of these eigenmodes together with the square of the first four wavefunctions. One can clearly see the excellent agreement for each $n \leq 3$ between the squared absolute value of the envelope of the mode and the squared wavefunction.

[^6]We can start quantifying the degree of agreement by comparing both frequency spacings. For


Figure 3.2: Comparison of the FDTD results with the probability distributions of the corresponding wavefunctions. Apart from the again plotted intensities of the first four eigenmodes, the squared absolute value of the first four wavefunctions of the quantum harmonic oscillator are depicted (red dashed). In the background the dielectric function $\varepsilon(x)$ (gray) of the PhC is plotted, its value indicated on the right axis.
that we have to admit that the frequency spacing between the electromagnetic modes as calculated by the FDTD simulations is not exactly constant, but slightly decreasing as can be concluded from Table 3.3.
We see that the spacing decreases for higher mode numbers, i.e. for the modes that are more spatially extended. These modes are still well localized inside the crystal and have negligible intensity at the boundary. They even do not reach the regions where the slab widths are smaller than 0.35 , but they do touch the boundary of the range of widths indicated in Figure 3.1. It also might have something to do with (one of) the approximations made in the MPB scheme: the width-energy relation is not perfectly linear and the effective mass obviously is not truly constant. This means that the potential deviates from being strictly harmonic.
Comparing these frequency spacings from Table 3.3 with the harmonic oscillator frequency 4.23 THz , that we inferred from the MPB calculations in combination with the quadratic chirping, we see that those differ by about $10 \%$.
As discussed in Section 2.2, we can determine the envelope of a mode if we know the loca-

| Mode number | Frequency $\left[\frac{c}{a}\right]$ |
| :--- | ---: |
| 0 | 0.29209 |
| 1 | 0.29846 |
| 2 | 0.30465 |
| 3 | 0.31077 |
| 4 | 0.31660 |
| 5 | 0.32237 |

Table 3.2: Frequencies of the first six modes found by a simulation using the parameter values given in Table 3.1.

| Mode numbers | Frequency difference $\left[\frac{c}{a}\right]$ | Frequency difference $[\mathrm{THz}]$ |
| :--- | :---: | ---: |
| $0-1$ | $6.37 \times 10^{-3}$ | 3.82 |
| $1-2$ | $6.19 \times 10^{-3}$ | 3.71 |
| $2-3$ | $6.12 \times 10^{-3}$ | 3.67 |
| $3-4$ | $5.83 \times 10^{-3}$ | 3.50 |
| $4-5$ | $5.77 \times 10^{-3}$ | 3.46 |

Table 3.3: Frequency differences between the modes mentioned in Table 3.2.
tion in momentum space of this mode, which resides at the bottom of the air band. In the one-dimensional case all the extrema of the bands lie at the edge of the irreducible BZ [15] and thus $\mathbf{k}_{\text {min }}=\frac{\pi}{a}$. Following the procedure explained in Section 2.2, which we schematically depict in Figure 3.3, we thus find the envelope $\psi_{m}$ for $m \in\{0,1, \ldots, 5\}$.
To quantify the agreement with the corresponding wavefunctions we will calculate the coefficient $c_{m, n}=\left\langle\psi_{m} \mid \phi_{n}\right\rangle$. However, by default Meep only outputs the real part of the electromagnetic field that it computes. Since we also want the absolute values of the modes and because the corresponding wavefunctions can be complex-valued, we need the imaginary part of the fields as well. One can easily change the default setting of Meep, but that doubles the amount of computation time, memory usage and storage space. A more efficient way is to realize that the FT from the time domain to the frequency domain of the real part of the magnetic field $\mathbf{H}(\mathbf{r}, t)$ can be written as

$$
\begin{equation*}
\tilde{\mathbf{H}}(\mathbf{r}, \omega)=\int_{t=-\infty}^{\infty} \mathbf{H}(\mathbf{r}, t) \cos (\omega t) \mathrm{dt} . \tag{3.5}
\end{equation*}
$$

Using Euler's formula we write this as

$$
\begin{equation*}
\frac{1}{2} \int_{t=-\infty}^{\infty} \mathbf{H}(\mathbf{r}, t)\left(e^{i \omega t}+e^{-i \omega t}\right) \mathrm{dt} \tag{3.6}
\end{equation*}
$$

If we now only integrate from $t=0$ until $t=\infty$, we have the following identity:

$$
\begin{equation*}
\frac{1}{2} \int_{t=0}^{\infty} \mathbf{H}(\mathbf{r}, t)\left(e^{i \omega t}+e^{-i \omega t}\right) \mathrm{dt}=\frac{1}{2} \int_{t=-\infty}^{\infty} \mathbf{H}(\mathbf{r}, t) e^{-i \omega t} \mathrm{dt} . \tag{3.7}
\end{equation*}
$$

By taking the inverse FT of this expression we thus retrieve the complex-valued magnetic field $\mathbf{H}(\mathbf{r}, t)$. We are now in the position to calculate the contributions $\left|c_{m, n}\right|^{2}$ of the wavefunctions $\phi_{n}$ to the envelope of the mode $\psi_{m}$. As an example, the results for the third envelope $\psi_{2}$ are


Figure 3.3: Obtaining the envelope of an eigenmode of the one-dimensional chirped PhC . In (a) the field (blue) of Figure 3.2(a) is again plotted for convenience. In (b) the spatial Fourier transform (blue) of this field is depicted. A mask (red dashed) is centered at the edge of the first BZ. Multiplying (b) with the complex conjugate of the corresponding plane wave and taking the inverse Fourier transorm results in the envelope (green dashed) in (c).
given in Figure 3.4. One can see that the contribution of the $3^{\text {rd }}$ wavefunction exceeds $90 \%$ while the others contribute very little. The envelopes of the lower modes $\psi_{m}$ show even higher contributions $\left|c_{m, m}\right|^{2}$ as shown in Table 3.4. The envelopes of the electromagnetic modes in a quadratically chirped PhC thus can, up to a large extend, be described by the wavefunctions of the one-dimensional quantum harmonic oscillator.
The results shown here for the chirping rate parameter $\eta=40 a$ should be seen as a proof of concept. However, decreasing the value of $\eta$ means that the local density approximation becomes less accurate. On the other hand, for large values of $\eta$ the eigenmode energies are smaller spaced apart and are (much) harder to excite using a single broad pulse. Also the computation time increases, as a larger $\eta$ implies a slower chirping and thus a larger PhC . The size of the crystal scales linearly with $\eta$ and is about $2 \sqrt{w_{\max }} \eta$.

### 3.1.4 One-dimensional distorted harmonic cavity

In contrast to the perfectly quadratically chirped PhCs discussed so far, PhCs that are fabricated in the real world suffer from all kinds of imperfections. Notably the widths and the

| Mode number $m$ | Contribution $\left\|c_{m, m}\right\|^{2}$ |
| :--- | ---: |
| 0 | $98.2 \%$ |
| 1 | $95.1 \%$ |
| 2 | $92.4 \%$ |
| 3 | $89.7 \%$ |
| 4 | $86.5 \%$ |
| 5 | $82.4 \%$ |

Table 3.4: For each $m \leq 5$ the contribution of the $m^{\text {th }}$ wavefunction to the envelope of the $m^{\text {th }}$ eigenmode of the one-dimensional perfect quadratically chirped PhC is given here.


Figure 3.4: Envelope of a single mode $\psi_{m}$ compared with the wavefunctions $\phi_{n}$ of the quantum harmonic oscillator. In (a) the envelope of $\psi_{2}$ is shown. From (b) until (e) the first four wavefunctions are depicted. In (f) the sum of the remaning higher harmonics is plotted. The contributions of these wavefunctions to $\psi_{2}$ are given in their respective upper right corners.

| Mode number $m$ | Contribution $\left\|c_{m, m}\right\|^{2}$ |
| :--- | ---: |
| 0 | $98.2 \%$ |
| 1 | $95.1 \%$ |
| 2 | $93.0 \%$ |
| 3 | $89.1 \%$ |
| 4 | $85.7 \%$ |
| 5 | $80.6 \%$ |

Table 3.5: For each $m \leq 5$ the contribution of the $m^{\text {th }}$ wavefunction to the envelope of the $m^{\text {th }}$ eigenmode of the one-dimensional distorted chirped PhC is given here.
positions of the dielectric slabs will acquire some distortions with respect to the desired values. Distortions of the latter kind do not influence the average local dielectric constant. The energy or frequency of a mode will therefore change only marginally. In the dispersion diagram this moving of the position of a slab amounts to moving a little bit in $k$-space. However, since we are at the minimum of the band, this has no effect on the energy of the mode up to first order in $k$.
Distortions on the slab widths do have a large impact on the modes. This is the case because the minimum of the air band is directly influenced by a change in the width, as can be inferred from Equation 3.1.
To take this into account in the simulations, we introduced a randomly generated distortion of the widths of the slabs, that before yielded a harmonic cavity. In that way Equation 3.2 now generalizes to

$$
\begin{equation*}
w(x)=w_{\max }-\left(\frac{x}{\eta}\right)^{2}+\Delta w(x) \tag{3.8}
\end{equation*}
$$

where $\Delta w(x)$ denotes the width distortion. This distortion is picked from a normal distribution with a standard deviation $\sigma_{w}$ of $10 \mathrm{~nm}^{17}$. A simulation with these widths results in the mode fields as depicted in Figure 3.5. We also want to test our model for this anharmonic effective potential. We can no longer rely on the analytical solutions of the quantum harmonic oscillator, but we have to numerically solve the one-dimensional Schrödinger equation using the induced distorted potential, and same $m^{*}$ as before. This can be achieved using a Numerov method [22-24], a derivation of which is given in Appendix C.
In Figure 3.5 we superimposed the numerical results on the modes we found in the FDTD simulations, we see that the agreement with the envelopes of the modes is very good. The contributions $\left|c_{m, m}\right|^{2}$ of the $m^{\text {th }}$ wavefunction to the $m^{\text {th }}$ envelope are given in Table 3.5. We thus have shown that our local density approach works not only in the case of a perfect harmonic cavity, but also when we introduced distortions on the slab widths of such a onedimensional chirped PhC .
We should note here that the agreement is, a bit suprisingly, worse (especially for the spatially larger modes) if we do not use the linear approximation between the slab width and energy (equation 3.1) but use the exact relation as depicted in Figure 3.1. This might be explained as

[^7]

Figure 3.5: FDTD results of the fields in a distorted harmonic potential. The intensity of the fields (blue) are plotted as a function of the position $x$ for the first four eigenmodes. In each plot, the numerically obtained wavefunctions (green dashed) are included. Each green
dot depicts a grid point used in the numerical solving method. In the background the dielectric function $\varepsilon(x)$ (gray) of the PhC is plotted, its value indicated on the right axis.
follows. These larger modes in fact experience a higher effective mass than the used average effective mass $m^{*}$ in the range of widths $0.35-0.45$. In the linear approximation this is compensated by a higher effective potential at smaller widths.

### 3.2 Two-dimensional harmonic cavity

As we plan to experimentally achieve a photonic BEC in a two-dimensional harmonic cavity, we shall now investigate the results for a two-dimensional quadratically chirped PhC . As explained in Chapter 2 we use a triangular lattice of air holes in a dielectric medium as our PhC , since the optical bandstructure of such a material exhibits a complete photonic bandgap for large enough hole sizes. In this section we will examine the correspondence between the wavefunctions
obtained using the local density approach and the electromagnetic modes resulting from the FDTD simulations in such a two-dimensional structure.

### 3.2.1 Effective mass and effective potential

Performing bandstructure calculations for PhCs with a varying air hole radius $\rho$, reveals that a clearly visible bandgap is apparent when this radius exceeds about $40.5 \%$ of the lattice parameter. The first band above the bandgap is the third TM-band for all structures with a large enough radius ${ }^{18}$. As for the one-dimensional structure we would like to find a relation between the hole size/radius and the effective mass and potential, which we can use to create a harmonic potential. The two-dimensionality of the system implies a possibly anisotropic effective mass as mentioned in Subsection 2.1.5. Fortunately it turns out that the effective mass is almost isotropic when calculated from the third TM-band at the location of the minimum of the band. This minimum appears to be practically at the K-point, which allows us to extract the effective mass from the bandstructure in two directions: In the direction of the $M$-point, the effective mass $m_{K M}^{*}$ equals $3.87 \mu m_{\mathrm{e}}$, where $m_{e}$ denotes the electron mass. In the direction of the $\Gamma$-point, $m_{K \Gamma}^{*}=4.08 \mu m_{\mathrm{e}}$. This amounts to a difference of only $5 \%$.
The relation between the hole radius and energy of the bottom of this band in the range $2 \rho \in[0.81,0.91]$ turns out to be again nearly linear as can be seen in Figure 3.6(a).
The effective masses $m_{K M}^{*}, m_{K \Gamma}^{*}$ are plotted in Figure 3.6(b) as a function of the air hole radius. Analogous to the one-dimensional case one thus should increase the hole size quadratically as a function of the distance to the crystal center to create a harmonic potential. In polar coordinates $r, \vartheta$ this is written as

$$
\begin{equation*}
\rho(r, \vartheta)=\rho(r)=\rho_{\min }+\frac{1}{2}\left(\frac{r}{\eta}\right)^{2} \tag{3.9}
\end{equation*}
$$

where $\rho_{\min }$ denotes the center hole radius. The resulting two-dimensional harmonic effective potential can be expressed by

$$
\begin{equation*}
V(r, \vartheta)=V(r)=\frac{1}{2} m^{*} \Omega^{2} r^{2} \tag{3.10}
\end{equation*}
$$

where $\Omega$ denotes the harmonic oscillator frequency and $m^{*}=\frac{1}{2}\left(m_{K M}^{*}+m_{K \Gamma}^{*}\right)$. Here $m_{K M}^{*}$ and $m_{K \Gamma}^{*}$ are both averaged over their values in the range $2 \rho \in[0.81,0.91]$.
We shall now look at the two-dimensional simulations results and how well they resemble the wavefunctions of a two-dimensional isotropic quantum harmonic oscillator.

### 3.2.2 FTDT and local density results

The parameters used for the two-dimensional simulation are given in Table 3.6. It turns out that for this simulation a resolution of 32 suffices as well. This means that the results from these simulations like the mode profiles only change very little upon increasing the resolution further. The simulation with a resolution of 64 took about 36 h per mode on a single core of

[^8]

Figure 3.6: MPB calculations for a range of hole radii $\rho$. In (a) the energy of the bottom of the third TM-band $E_{\min }(w)$ (red circles) is depicted. A first order polynomial (blue) is fitted to the data points that lie within the range depicted by the two vertical black dashed lines. In (b) the effective masses $m_{K M}^{*}, m_{K \Gamma}^{*}$ are indicated by green squares and purple triangles, respectively.
an Intel Core i3-2130 processor ${ }^{19}$. As explained in the case of the one-dimensional simulations in Subsection 3.1.3, the real-valued resulting fields have to be extended with their imaginary parts.
The intensities of the first four modes, together with the dielectric function, are plotted in Figure 3.7.
Again, as in the one-dimensional case, we want to extract the envelope function $\psi_{m}(r, \vartheta)$ from each of these modes. The procedure to do this, already described for the general case, is also schematically depicted in Figure 3.8 for the two-dimensional case. Here it is clearly visible that the fundamental mode is mostly located around the six K-points in the first BZ in momentum space.
To compare these envelopes with the analytical solutions to the corresponding Schrödinger equation, we have to investigate these solutions in some detail. This has been done in Ap-

[^9]| Parameter | Value |
| :--- | ---: |
| $a$ | 500 nm |
| $\eta$ | $40 a$ |
| $\rho_{\min }$ | 0.405 |
| resolution | $64 \frac{\mathrm{px}}{a}$ |
| $f_{\Delta}$ | $0.05 \frac{c}{a}$ |
| $f_{\text {cen }}$ | $0.4 \frac{c}{a}$ |
| $f_{\delta}$ | $0.001 \frac{c}{a}$ |
| excitation point | $(-1.775 a,-1.04482 a)$ |

Table 3.6: Parameters used for the simulation of electromagnetic modes in a two-dimensional chirped PhC .


Figure 3.7: FDTD results of the fields in two dimensions. From white to dark red, the intensity of the fields are depicted for the first four eigenmodes. On top of these fields, the chirped PhC is plotted, where the dielectric material is shown in black and the air holes in white.
pendix D . These wavefunctions $\phi_{n, l}$, where $n$ is the principal quantum number that determines the energy and the quantum number $l$ determines the z-component of the orbital angular momentum, are given in Equation D.18. They are here restated for convenience

$$
\begin{equation*}
\phi_{n, l}(r, \vartheta)=C_{n, l} e^{-\left(r / 1_{\mathrm{HO}}\right)^{2} / 2}\left(r / \mathrm{l}_{\mathrm{HO}}\right)^{|l|} L_{\frac{n-|l|}{2}}^{|l|}\left(\left(r / \mathrm{l}_{\mathrm{HO}}\right)^{2}\right) e^{i l \vartheta} \tag{3.11}
\end{equation*}
$$

where $L_{p}^{l}(\zeta)$ the generalized Laguerre polynomials and $C_{n, l}=1_{\mathrm{HO}}^{-1} \sqrt{\frac{2 p!}{(p+|l|)!}}$ a normalization constant, with $p=\frac{n-|l|}{2}$. Each energy level $n$ is $(n+1)$-fold degenerate.
For each of these wavefunctions $\phi_{n, l}$ the coefficient $c_{m,\{n, l\}}$ in the expansion of the envelope


Figure 3.8: Obtaining the envelope of an eigenmode of the two-dimensional chirped PhC . In (a) the intensity of the field of Figure 3.7(a) is again plotted for convenience. In (b) the spatial Fourier transform of this field is depicted. A mask (blue dashed) is placed around an intensity maximum (here centered at the third $K$-point). Applying this mask results in (c). Multiplying (c) with the complex conjugate of the corresponding plane wave and taking the inverse Fourier transform results in the envelope in (d).
$\psi_{m}$ of the electromagnetic mode found in the FDTD simulations can be calculated as

$$
\begin{equation*}
c_{m,\{n, l\}}=\left\langle\psi_{m} \mid \phi_{n, l}\right\rangle . \tag{3.12}
\end{equation*}
$$

We can then form for a certain energy (frequency) level $n$ the total wavefunction

$$
\begin{equation*}
\phi_{n}=\sum_{l} c_{m,\{n, l\}} \phi_{n, l} . \tag{3.13}
\end{equation*}
$$

The contribution $\left|c_{m, n}\right|^{2}$ of this wavefunction to the envelope can be computed using $\left|c_{m, n}\right|^{2}=$ $\sum_{l}\left|c_{m,\{n, l\}}\right|^{2}$.
In Figure 3.9 the contributions to the third envelope (which itself is depicted in the upper left corner) are given and the corresponding $\phi_{n}$ for $n \in\{0, \ldots, 5\}$ are shown. We find a good agreement between the third envelope and third harmonic oscillator wavefunction: $\left|c_{2,2}\right|^{2}=$ $92.0 \%$, when we used the upper right $K$-point in the demodulation procedure to find the envelope $^{20}$. For the lower envelopes even higher values are found. For higher $m,\left|c_{m, m}\right|^{2}$ slowly decreases as the harmonic oscillator approximation deteriorates for the larger modes. ${ }^{21}$

[^10]For completeness, all the contributions $\left|c_{m, m}\right|^{2}$ for $m \leq 5$ and for all pairs of $K$-points in the first BZ are listed in Table 3.7. We cannot yet attribute the differences between the contributions when varying the $K$-point used in obtaining the envelopes, but we can note here there seems to be some relation with the position of the excitation point. However, increasing the pulse durations in the simulations does not alter the values in Table 3.7. In this table, the contributions for the higher modes in fact are not exactly equal for opposing $K$-points, which is in contradiction with the time-reversal symmetry of the modes. For a complete understanding of these issues concerning the higher modes further investigation is thus needed.

| Mode number $m$ | Contribution $\left\|c_{m, m}\right\|^{2}$ |  |  |
| :---: | :---: | :---: | :---: |
|  | $K$-points 1,4 | $K$-points 2,5 | $K$-points 3,6 |
| 0 | $99.1 \%$ | $98.9 \%$ | $98.9 \%$ |
| 1 | $96.9 \%$ | $98.1 \%$ | $92.7 \%$ |
| 2 | $96.1 \%$ | $89.1 \%$ | $92.0 \%$ |
| 3 | $91.2 \%$ | $94.4 \%$ | $81.1 \%$ |
| 4 | $89.3 \%$ | $72.4 \%$ | $84.9 \%$ |
| 5 | $87.4 \%$ | $80.9 \%$ | $80.2 \%$ |

Table 3.7: For each $m \leq 5$ and each pair of opposing $K$-points used in the process to obtain the envelop of a mode (see Figure 3.8), the contribution of the $m^{\text {th }}$ wavefunction to the envelope of the $m^{\text {th }}$ eigenmode of the two-dimensional chirped PhC is given here. See Footnote 20 for the assignment of the $K$-point numbers.


Figure 3.9: Envelope of a single mode $\psi_{m}$ compared with the wavefunctions $\phi_{n}$ of the quantum harmonic oscillator. In (a) the envelope of $\psi_{2}$ is shown. From (b) until (g) the first six wavefunctions are depicted. In (h) the sum of the remaning higher harmonics is plotted. The contributions of these wavefunctions to $\psi_{2}$ are given in their respective upper right corners.

## 4 Conclusion

The intuitive model described in this thesis, where a slowly chirped PhC is modeled as an effective potential for a massive boson and the envelopes of eigenmodes are found by solving the corresponding Schrödinger equation, has been shown to be very accurate. For the treated one- and two-dimensional harmonic cavities, the agreements between the lowest eigenmodes and their corresponding analytical wavefunctions have been shown to be higher than $90 \%$. The distorted one-dimensional case also exhibited qualitatively similar results. This accuracy is surprisingly good, especially when one keeps in mind that the time needed to calculate the envelopes in this novel model is many orders of magnitude smaller than the time it takes to simulate them using an FDTD approach.
The limits of the validity of this model have not been fully exploired yet, but it is clear from Figures 3.1 and 3.6 that the model works better in some ranges of hole/slab sizes than in others. It tends to be less accurate when a larger range of air holes/slabs is covered by the modes under consideration.
It can be also expected that the local density approximation becomes less accurate if the hole/slab size is changed too rapidly.
Keeping in mind that the boundaries of the validity of the model are not precisely known at the moment, it can be of great interest when designing large PhCs , for example in the field of solid-state lighting.

## 5 Outlook

In this thesis the electromagnetic modes in a large area quadratically chirped PhC were described. In particular the novel model that we discussed to calculate the envelopes of these modes has been investigated in great detail. This was just the first part of larger project in which we plan to create a Bose condensed photon gas. The next step to reach this goal is to perform FDTD simulations in which the quadraticaly chirped PhC is replaced by the very same crystal, except that it has to be modified in such a way that an incoming electromagnetic wave, originating from a laser source, can be coupled in and out the PhC. The optimal design of this crystal is one of the first challenges ahead. When the eigenmodes of this new structure are known, the actual experimental design (semiconductor material, thickness, etc.) and fabrication of the PhCs can be taken up. This will be a formidable achievement in itself, when one takes into account the extremely thin dielectric material that constitutes the crystal. Subsequently a designated laser will pump the crystal, which partly absorbs and re-emits these photons and thereby allowing them to thermalize, and will hopefully form a photonic BEC with an energy just above the optical bandgap of the corresponding periodic PhC.
If this succeeds, the periodicity of the structure can be more exploited. A similar approach has been taken in the field of atomic BECs where a periodic potential over the condensate can be created using opposing laser beams, thereby creating an optical lattice [25,26].
By tuning several experimental parameters, large non-linear effects in the PhC are expected to occur and thereby opening the way to describe the photonic BEC in the periodic potential by the Bose-Hubbard model. In this way we hope to make a quantum phase transition from the superfluid BEC state to a Mott-insulator state with a small integer number of photons per unit cell.
These fascinating challenges are not only of fundamental interest but may also imply applications in the field of quantum information and novel PhC LEDs.

## 6 Acknowledgements

The past year I had a great, interesting and challenging time in the Nanophotonics group of the Utrecht University.
First of all, I would like to thank Jaap Dijkhuis and Dries van Oosten for their enthusiastic talks when I came by to be informed about potential subjects for a master thesis, despite the fact that I had entered the master via a bachelor in chemistry. After the summer holidays I quickly felt really part of the Nanophotonics section and the group led by Dries in particular. It was an honour to be part of this group.
I am very grateful to Dries for his energetic, enthusiastic and honoust way of supervising. Apart from all the questions you answered me, I now particularly would like to thank you for writing a recommendation letter for my potential employers during your own holiday.
I also would like to express my gratitude to my daily supervisor and former fellow student Sebastiaan Greveling for all his cordial and patient $24 / 7$ help with all my physics and programming problems(/challenges). I will remember our intensive teamwork as fruitful and pleasant and without you the figures in this thesis certainly would not be as beautiful as they are now. Furthermore, I thank you for carefully pre-reading this manuscript twice.
I wish you both the best of luck with the photonic BEC experiment and I am really curious about the upcoming results.
The other PhD students of our group Arjon van Lange, Ole Mussmann and Sandy Pratama, I'd like to thank for all the lunch breaks we spent together and the usefull discussions, of all kinds, we had.
After being encouraged by Dries, I have written a PhD proposal for combined research inside the Debye Institute for Nanomaterials Science. During this process I cooperated with Peter van der Straten and Daniël Vanmaekelbergh, which was my pleasure and for which I would like to acknowledge them. Unfortunately the proposal was not selected to be funded. I furthermore want to thank Peter for being the second examiner of my master project.
I also would like to mention the rest of the (former) students of our subgroup Zimma Kluit, Bas Meyer Viol, Gilian van den Hengel and Michel Ram for their agreeable company and good times during some months of the past year. I had far less contact with most of the students working on atomic BECs, but I also would like to thank them for the friendly discussions we had. In particular I want to acknowledge Chris(tian) te Riet for the numerous interesting conversations we had and for your endless enthusiasm.
Last, but not least, I am deeply indebted to my parents Joke and Paul Dobbelaar who made my education switch possible and kept supporting me all these years.

## Appendix A Software

For the bandstructure calculations the open source software package MIT Photonic Bands (MPB) was employed. This package involves an iterative eigensolver algorithm that solves Maxwell's equations for periodic structures in a plane-wave basis [27]. It thus tries to find eigenmodes of Equation 2.6, under the restriction of the divergenceless of the $\mathbf{H}$-field.
To find the electromagnetic eigenmodes of non-periodic structures using finite-difference timedomain (FDTD) simulations, we invoked another open source program developed at MIT: Meep [28]. This acronym officially stands for MIT Electromagnetic Equation Propagation. This software package solves Maxwell's equation in the time-domain and lets them evolve for some small time-interval and using a fine computational grid.
To determine the frequency components of electromagnetic fields the accompanying free program Harminv was exploited. For more information about this method, see for instance Mandelshtam et al. [29, 30].
At the edges of a finite computational region so-called perfectly matched layers (PMLs) can be defined. These artificial layers are supposed to absorb any light that enters $\mathrm{it}^{22}$ and thus represents an empty space surrounding the in silico structure. The electromagnetic modes that are discussed in this thesis all have a negligible intensity outside the considered PhC and thus in the PML.

[^11]
## Appendix B Units

The MIT software has not adopted the SI-unit system. Therefore one often has to convert the output of calculations to numbers in more conventional units. We therefore spend here some words on the scale-invariant MIT units and on how to convert them to SI-units.
In the units utilized by the MIT software the speed of light in vacuum $c$, the vacuum permittivity $\varepsilon_{0}$ and vacuum permeability $\mu_{0}$ are put to 1 . Furthermore the lattice constant $a$ is also defined to be 1 . If we, for instance, encounter a frequency of $f=0.3$ and set $a$ equal to $0.5 \mu \mathrm{~m}$, this frequency equals $0.3 \frac{c}{a} \approx 180 \mathrm{THz}$ in SI-units. Wavevectors are treated differently in Meep in comparison with MPB. In MPB these are given in a basis of reciprocal lattice vectors. In Meep they are expressed in rectangular coordinates, in units of $\frac{2 \pi}{a}$. Here an example is provided which exhibits how to work with these units. Assume we have obtained a dispersion diagram using MPB and we want to assign an effective mass $m^{*}$ to photons residing in the air band of the periodic structure used in the calculation. We thus intend to use Equation 2.13, which is here conveniently displayed again

$$
\begin{equation*}
E(\mathbf{k})=E\left(\mathbf{k}_{\min }\right)+\frac{\hbar^{2}}{2 m^{*}}\left(\mathbf{k}-\mathbf{k}_{\min }\right)^{2} . \tag{B.1}
\end{equation*}
$$

As we are now only interested in the unit conversion factor for the effective mass, we can forget about the constant energy term and put $\mathbf{k}_{\min }$ also equal to 0 . We then divide the remaining equation by Planck's constant to obtain

$$
\begin{equation*}
f(\mathbf{k})=\frac{h}{2 m^{*}(2 \pi)^{2}} \mathbf{k}^{2} \tag{B.2}
\end{equation*}
$$

We can now extract the factor $\frac{c}{a}$ out of the frequency $f$ and $\frac{2 \pi}{a}$ out of the wavevector $\mathbf{k}$, as to convert the SI-units to MIT-units (as to correspond to the output of the software). Moving the frequency factor to the right, results in

$$
\begin{equation*}
f(\mathbf{k})=\frac{h}{2 m^{*} a c} \mathbf{k}^{2} \tag{B.3}
\end{equation*}
$$

If we fit the dispersion around $\mathbf{k}_{\min }(=0)$, we find that the coefficient $\zeta$ of the quadratic term in $\mathbf{k}$ thus equals

$$
\begin{equation*}
\zeta=\frac{h}{2 m^{*} a c} . \tag{B.4}
\end{equation*}
$$

Since we know $\zeta$ from the fit, we can now express $m^{*}$ in MPB output as

$$
\begin{equation*}
m^{*}=\frac{h}{2 \zeta a c m_{e}} \tag{B.5}
\end{equation*}
$$

where we have also divided by the electron mass $m_{e}$.

## Appendix C Normalized Numerov integration method

The Numerov method is an efficient algorithm for solving second order linear differential equations in one dimension that does not involve a first order term ${ }^{23}$. We can thus use it to solve the one-dimensional Schrödinger equation

$$
\begin{equation*}
\frac{\mathrm{d}^{2} \phi(x)}{\mathrm{d} x^{2}}+k^{2} \phi(x)=0 \tag{C.1}
\end{equation*}
$$

where we have defined $k^{2}$ as $\frac{2 m^{*}}{\hbar^{2}}(E-V(x))$.
In order to numerically solve this equation for some given potential $V(x)$, it is necessary to discretize the one-dimensional space. This is achieved using equidistant points $x_{i}$ and we define $h$ to be the stepsize $x_{i+1}-x_{i}$.
Let us now assume that we can Taylor expand a solution $\phi$ of the Schrödinger equation around $x_{i}$, such that

$$
\begin{equation*}
\phi\left(x_{i+1}\right)=\phi\left(x_{i}\right)+h \phi^{\prime}\left(x_{i}\right)+\frac{h^{2}}{2} \phi^{\prime \prime}\left(x_{i}\right)+\frac{h^{3}}{3!} \phi^{(3)}\left(x_{i}\right)+\frac{h^{4}}{4!} \phi^{(4)}\left(x_{i}\right)+\mathcal{O}\left(h^{5}\right), \tag{C.2}
\end{equation*}
$$

where the $\mathcal{O}$ notation means that the error $\mathcal{R}_{5}\left(h, x_{i}\right)$ made by this approximation obeys

$$
\begin{equation*}
\limsup _{h \rightarrow 0}\left|\frac{\mathcal{R}_{5}\left(h, x_{i}\right)}{h^{5}}\right|<\infty \tag{C.3}
\end{equation*}
$$

If we use the shorthand notation of denoting $\phi\left(x_{i}\right)$ by $\phi_{i}$ and similarly for the derivatives, we can also write

$$
\begin{equation*}
\phi_{i-1}=\phi_{i}-h \phi_{i}^{\prime}+\frac{h^{2}}{2} \phi_{i}^{\prime \prime}-\frac{h^{3}}{3!} \phi_{i}^{(3)}+\frac{h^{4}}{4!} \phi_{i}^{(4)}+\mathcal{O}\left(h^{5}\right) \tag{C.4}
\end{equation*}
$$

and thus

$$
\begin{equation*}
\phi_{i+1}+\phi_{i-1}=2 \phi_{i}+h^{2} \phi_{i}^{\prime \prime}+\frac{h^{4}}{12} \phi_{i}^{(4)}+\mathcal{O}\left(h^{6}\right) . \tag{C.5}
\end{equation*}
$$

We now want to find expressions for these higher order derivatives in terms of $\phi$ itself. Since $\phi$ obeys the Schrödinger equation we know that its second derivative equals $-k^{2} \phi$, so that

$$
\begin{equation*}
\phi_{i}^{(4)}=-\left(k^{2} \phi_{i}\right)^{\prime \prime} . \tag{C.6}
\end{equation*}
$$

Furthermore, the first derivative $\phi_{i}^{\prime}$ can be approximated by

$$
\begin{equation*}
\phi_{i}^{\prime}=\frac{\phi_{i+\frac{1}{2}}-\phi_{i-\frac{1}{2}}}{h} \tag{C.7}
\end{equation*}
$$

where we have generalized the shorthand notation by writing $\phi_{i+\frac{1}{2}}$ instead of $\phi\left(x_{i}+\frac{h}{2}\right)$. Taking the derivative of this expression yields

$$
\begin{equation*}
\phi_{i}^{\prime \prime}=\frac{\phi_{i+\frac{1}{2}}^{\prime}-\phi_{i-\frac{1}{2}}^{\prime}}{h} \tag{C.8}
\end{equation*}
$$

which, using Equation C.7, can be rewritten as

$$
\begin{equation*}
\phi_{i}^{\prime \prime}=\frac{\left(\phi_{i+1}-\phi_{i}\right)-\left(\phi_{i}-\phi_{i-1}\right)}{h^{2}} . \tag{C.9}
\end{equation*}
$$

$\overline{{ }^{23} \text { Our main reference for this section is Van }}$ der Zwan [24].

This leads, together with Equation C. 6 to

$$
\begin{equation*}
h^{2} \phi_{i}^{(4)}=-k_{i+1}^{2} \phi_{i+1}+2 k_{i}^{2} \phi_{i}-k_{i-1}^{2} \phi_{i-1} . \tag{C.10}
\end{equation*}
$$

This means we can rewrite Equation C. 5 (neglecting the rest term) as

$$
\begin{equation*}
\left(1-T_{i+1}\right) \phi_{i+1}-\left(2+10 T_{i}\right) \phi_{i}+\left(1-T_{i-1}\right) \phi_{i-1}=0 \tag{C.11}
\end{equation*}
$$

where we have used the common notation $T_{i}:=-\frac{1}{12} h^{2} k_{i}^{2}$. This three-point equation we would like to convert into a two-point equation, i.e. we want to employ the faster normalized Numerov method.
If we define $F_{i}:=\left(1-T_{i}\right) \phi_{i}$ and $U_{i}:=\frac{2+10 T_{i}}{1-T_{i}}$ we can write Equation C. 11 conveniently as

$$
\begin{equation*}
F_{i+1}-U_{i} F_{i}+F_{i-1}=0 . \tag{C.12}
\end{equation*}
$$

Now we are in the right position to proceed to the normalized setting, by defining $R_{i}:=\frac{F_{i+1}}{F_{i}}$ and thereby allowing us to write the resulting two-point equation

$$
\begin{equation*}
R_{i}=U_{i}-\frac{1}{R_{i-1}} \tag{C.13}
\end{equation*}
$$

Or starting the integration from the other side one can obtain analogously

$$
\begin{equation*}
\tilde{R}_{i}=U_{i}-\frac{1}{\tilde{R}_{i+1}}, \tag{C.14}
\end{equation*}
$$

where $\tilde{R}_{i}:=R_{i-1}^{-1}$. One can then reconstruct the wavefunction by using the definitions given above to obtain the following relations

$$
\begin{align*}
\phi_{i+1} & =\frac{\left(1-T_{i}\right) R_{i}}{\left(1-T_{i+1}\right)} \phi_{i} \\
\phi_{i-1} & =\frac{\left(1-T_{i}\right) \tilde{R}_{i}}{\left(1-T_{i-1}\right)} \phi_{i} \tag{C.15}
\end{align*}
$$

Because of the existence of non-physical solutions which are not normalizable, this does not give the desired wavefunction yet. In an unnormalized Numerov method one starts the integration procedure from both sides on, until they meet in the middle of the computational grid. After multiplying one of them by a constant (the Numerov algorithm and the Schrödinger equation are linear in the solutions $\phi$ ), they can always be made to concide in the center. The real test whether they constitute a real wavefunction is whether their derivatives are equal at the meeting point $x_{n}$. To ensure the independency on the absolute value at this point, we thus want to find a root of the function $D(E)$ that takes the difference of the two logarithmic derivatives $y_{n}^{+}$and $y_{n}^{-}$of the two constructed $\phi$ at $x_{n}$.
For the normalized scheme, we approximate the logarithmic derivative $\frac{\phi_{i}^{\prime}}{\phi_{i}}$ by $\frac{F_{i}^{\prime}}{F_{i}}$, which is the most accurate when the potential varies slowly in space ${ }^{24}$. This fraction can, again, be numerically approximated by $\frac{F_{i+1}-F_{i}}{h F_{i}}$, so that we have $R_{i}=1+y_{i}^{+}$and similarly $\tilde{R}_{i+1}^{-1}=1+y_{i}^{-}$. This means that finding a root of the function $D(E)$ is translated into finding a zero of

$$
\begin{equation*}
R_{n} \tilde{R}_{n+1}-1 \tag{C.16}
\end{equation*}
$$

If this condition is fullfilled, an eigenvalue $E$ of the Hamiltonian is found and a wavefunction can be built up using the $R_{i}, U_{i}$ and $F_{i}$ after setting $R_{0}$ and $F_{0}$ to small starting values.

[^12]
## Appendix D Two-dimensional isotropic quantum harmonic oscillator

In this appendix the solutions to the two-dimensional isotropic quantum harmonic oscillator are investigated. The two main references for this section are Cohen-Tannoudji et al. [33] and Karimi et al. [34].
In cartesian coordinates the Schrödinger equation of this harmonic oscillator is written as

$$
\begin{equation*}
\left\{-\frac{\hbar^{2}}{2 m}\left(\frac{\partial^{2}}{\partial x^{2}}+\frac{\partial^{2}}{\partial y^{2}}\right)+\frac{1}{2} m \omega^{2}\left(x^{2}+y^{2}\right)\right\} \phi(x, y)=E \phi(x, y) \tag{D.1}
\end{equation*}
$$

where $m$ denotes the mass and E the energy of the particle that is described by the wavefunction $\phi$. $\omega$ denotes the harmonic oscillator frequency. A natural starting point in solving this equation is to use the method of separation of variables. It can then be easily seen that the wavefunction is just the product of two wavefunctions that are solutions to the one-dimensional Schrödinger equation with a harmonic oscillator potential, i.e. $\phi_{n_{x}, n_{y}}(x, y)=\phi_{n_{x}}(x) \phi_{n_{y}}(y)$ with energy $E_{n_{x}, n_{y}}=E_{n_{x}}+E_{n_{y}}$. Here $n_{i}$, with $i \in\{x, y\}$, denotes an integer that indexes the discrete solutions with energy $E_{n_{i}}$ of the quantum harmonic oscillator problem. These wavefunctions are given by Equation 3.3 and their respective energies in Equation 3.4. By defining the annihilation operator [35]

$$
\begin{equation*}
\hat{a}_{x}^{\dagger}:=\sqrt{\frac{m \omega}{2 \hbar}}\left(\hat{x}-\frac{i}{m \omega} \hat{p}\right), \tag{D.2}
\end{equation*}
$$

where a hat above an observable denotes the corresponding operator, and $\hat{p}=-i \hbar \frac{\mathrm{~d}}{\mathrm{~d} \hat{x}}$ the momentum operator. The creation operator $\hat{a}_{x}$ is defined as its hermitian conjugate. For the two-dimensional harmonic oscillator the operator $\hat{a}_{y}$ and its hermitian conjugate are defined in the same manner. The following relations between the consecutive wavefunctions can then be deduced

$$
\begin{align*}
\hat{a}_{x} \phi_{n}(x) & =\sqrt{n} \phi_{n-1}(x) \\
\hat{a}_{x}^{\dagger} \phi_{n}(x) & =\sqrt{n+1} \phi_{n+1}(x) \tag{D.3}
\end{align*}
$$

and analogous equations for the $\phi_{n_{y}}(y)$. We are now in the position to define the number operators $\hat{N}_{x}=\hat{a}_{x}^{\dagger} \hat{a}_{x}$ and $\hat{N}_{y}=\hat{a}_{y}^{\dagger} \hat{a}_{y}$, so that the hamiltonian $H_{x, y}$ can be written as $\hbar \omega\left(\hat{N}_{x}+\hat{N}_{y}+1\right)$. Furthermore the wavefunction $\phi_{n_{x}, n_{y}}$ is an eigenfunction of $\hat{N}_{x}$ and $\hat{N}_{y}$ with eigenvalues $n_{x}$ and $n_{y}$, respectively. One thus speaks of having $n_{x}$ quanta of light in the $x$ direction and $n_{y}$ quanta in the $y$ direction.
The wavefunction $\phi_{n_{x}, n_{y}}$ can thus be built up from the lowest energy wavefunction $\phi_{0,0}$ by letting the creation operators repeatedly operating on $\phi_{0,0}$

$$
\begin{equation*}
\phi_{n_{x}, n_{y}}=\frac{1}{\sqrt{n_{x}!n_{y}!}}\left(\hat{a}_{x}^{\dagger}\right)^{n_{x}}\left(\hat{a}_{y}^{\dagger}\right)^{n_{y}} \phi_{0,0} . \tag{D.4}
\end{equation*}
$$

Note that the states with an energy $E_{n_{x}+n_{y}}^{\mathrm{tot}}:=E_{n_{x}, n_{y}}$ are $\left(n_{x}+n_{y}\right)$-fold degenerate.
Since we assume that the potential landscape and the mass $m$ are isotropic, the axes $x$ and $y$ do not enjoy a privileged rôle and we should exploit this rotational symmetry around the z-axis. It is therefore natural to look at the z-component of the angular momentum $L_{z}$, which is classicaly defined by

$$
\begin{equation*}
L_{z}=x p_{y}-y p_{x} \tag{D.5}
\end{equation*}
$$

i.e. it is the last component of $(x, y, z)^{t} \times\left(p_{x}, p_{y}, p_{z}\right)^{t}$.

Since

$$
\begin{align*}
\hat{x} & =\sqrt{\frac{\hbar}{2 m \omega}}\left(\hat{a}_{x}^{\dagger}+\hat{a}_{x}\right),  \tag{D.6}\\
\hat{p}_{x} & =i \sqrt{\frac{\hbar m \omega}{2}}\left(\hat{a}_{x}^{\dagger}-\hat{a}_{x}\right),
\end{align*}
$$

and similarly for their $y$-equivalents, we can write $L_{z}$ as

$$
\begin{equation*}
L_{z}=i \hbar\left(\hat{a}_{x} \hat{a}_{y}^{\dagger}-\hat{a}_{x}^{\dagger} \hat{a}_{y}\right) \tag{D.7}
\end{equation*}
$$

As $\left[\hat{a}_{i}, \hat{a}_{j}^{\dagger}\right]=\delta_{j}^{i}$ for $i, j \in\{x, y\}$, we deduce the important commutation relation

$$
\begin{equation*}
\left[H_{x, y}, L_{z}\right]=0 \tag{D.8}
\end{equation*}
$$

Let us now define the two convenient operators

$$
\begin{equation*}
\hat{a}_{ \pm}=\frac{1}{\sqrt{2}}\left(\hat{a}_{x} \mp i \hat{a}_{y}\right) \tag{D.9}
\end{equation*}
$$

and their hermitian conjugates

$$
\begin{equation*}
\hat{a}_{ \pm}^{\dagger}=\frac{1}{\sqrt{2}}\left(\hat{a}_{x}^{\dagger} \pm i \hat{a}_{y}^{\dagger}\right) \tag{D.10}
\end{equation*}
$$

Again, the commutators obey the relations $\left[\hat{a}_{i}, \hat{a}_{j}^{\dagger}\right]=\delta_{j}^{i}$ for $i, j \in\{+,-\}$. It is also readily verified that $2 \hat{a}_{ \pm}^{\dagger} \hat{a}_{ \pm}=\hat{a}_{x}^{\dagger} \hat{a}_{x}+\hat{a}_{y}^{\dagger} \hat{a}_{y} \mp i \hat{a}_{x}^{\dagger} \hat{a}_{y} \pm i \hat{a}_{x} \hat{a}_{y}^{\dagger}$, so that we can write the hamiltonian and the z-component of the angular momentum as

$$
\begin{align*}
H_{x, y} & =\hbar \omega\left(\hat{a}_{+}^{\dagger} \hat{a}_{+}+\hat{a}_{-}^{\dagger} \hat{a}_{-}+1\right), \\
L_{z} & =\hbar\left(\hat{a}_{+}^{\dagger} \hat{a}_{+}-\hat{a}_{-}^{\dagger} \hat{a}_{-}\right) . \tag{D.11}
\end{align*}
$$

By using the operators $\hat{N}_{+}=\hat{a}_{+}^{\dagger} \hat{a}_{+}$and $\hat{N}_{-}=\hat{a}_{-}^{\dagger} \hat{a}_{-}$, we can write Equation D. 11 more compactly as

$$
\begin{align*}
H_{x, y} & =\hbar \omega\left(\hat{N}_{+}+\hat{N}_{-}+1\right),  \tag{D.12}\\
L_{z} & =\hbar\left(\hat{N}_{+}-\hat{N}_{-}\right)
\end{align*}
$$

The operator $\hat{N}_{-}\left(\hat{N}_{+}\right)$can be interpreted as the number of (counter)clockwise rotating quanta, i.e. the number of quanta with a negative (positive) orbital angular momentum around the $z$ axis.
The eigenvalues of these operators are denoted by $n_{+}, n_{-} \in \mathbb{N}_{0}$ and their common eigenfunctions can be, analogous to Equation D.4, constructed as

$$
\begin{equation*}
\phi_{n_{+}, n_{-}}=\frac{1}{\sqrt{n_{+}!n_{-}!}}\left(\hat{a}_{+}^{\dagger}\right)^{n_{+}}\left(\hat{a}_{-}^{\dagger}\right)^{n_{-}} \phi_{0,0} \tag{D.13}
\end{equation*}
$$

From Equation D. 12 we can conclude that these are also eigenfunctions of the hamiltonian and $L_{z}$, with the respective eigenvalues $\hbar \omega(n+1)$ and $\hbar l$, where $n=n_{+}+n_{-}$and $l=n_{+}-n_{-}$. Given an energy of $\hbar \omega(n+1)$ and the relation $l=n-2 n_{-}$, we see that the $(n+1)$-fold degeneracy can here be expressed by noting that $l$ can have the values $n, n-2, \ldots, 2-n,-n$. To acquire explicit expressions for the operators $\hat{a}_{ \pm}$and $\hat{a}_{ \pm}^{\dagger}$ in the polar coordinates

$$
\begin{align*}
& x=\rho \cos \vartheta \\
& y=\rho \sin \vartheta \tag{D.14}
\end{align*}
$$

we first write the operators as functions of cartesian coordinates. For example, we find for $\hat{a}_{+}$

$$
\begin{equation*}
\hat{a}_{+}=\frac{1}{2}\left\{\sqrt{\frac{m \omega}{\hbar}}(x-i y)+\sqrt{\frac{\hbar}{m \omega}}\left(\frac{\partial}{\partial x}-i \frac{\partial}{\partial y}\right)\right\} . \tag{D.15}
\end{equation*}
$$

By using the inverse of the Jacobian matrix of the coordinate transformation to polar coordinates and Euler's formula, we arrive at

$$
\begin{equation*}
\hat{a}_{+}=\frac{e^{-i \vartheta}}{2}\left\{\sqrt{\frac{m \omega}{\hbar}} \rho+\sqrt{\frac{\hbar}{m \omega}}\left(\frac{\partial}{\partial \rho}-\frac{i}{\rho} \frac{\partial}{\partial \vartheta}\right)\right\} . \tag{D.16}
\end{equation*}
$$

The others can be constructed in a similar fashion and are listed below

$$
\begin{align*}
& \hat{a}_{+}^{\dagger}=\frac{e^{i \vartheta}}{2}\left\{\sqrt{\frac{m \omega}{\hbar}} \rho-\sqrt{\frac{\hbar}{m \omega}}\left(\frac{\partial}{\partial \rho}-\frac{i}{\rho} \frac{\partial}{\partial \vartheta}\right)\right\}, \\
& \hat{a}_{-}=\frac{e^{i \vartheta}}{2}\left\{\sqrt{\frac{m \omega}{\hbar}} \rho+\sqrt{\frac{\hbar}{m \omega}}\left(\frac{\partial}{\partial \rho}+\frac{i}{\rho} \frac{\partial}{\partial \vartheta}\right)\right\},  \tag{D.17}\\
& \hat{a}_{-}^{\dagger}=\frac{e^{-i \vartheta}}{2}\left\{\sqrt{\frac{m \omega}{\hbar}} \rho-\sqrt{\frac{\hbar}{m \omega}}\left(\frac{\partial}{\partial \rho}-\frac{i}{\rho} \frac{\partial}{\partial \vartheta}\right)\right\} .
\end{align*}
$$

This leads to the following expression for the eigenfunctions indexed by the energy $n$ and the orbital momentum $l$

$$
\begin{equation*}
\phi_{n, l}(\rho, \vartheta)=C_{n, l} e^{-\left(\rho / l_{\mathrm{HO}}\right)^{2} / 2}\left(\rho / \mathrm{l}_{\mathrm{HO}}\right)^{|l|} L_{\frac{n-|l|}{2}}^{|l|}\left(\left(\rho / \mathrm{l}_{\mathrm{HO}}\right)^{2}\right) e^{i l \vartheta} \tag{D.18}
\end{equation*}
$$

where $\mathrm{l}_{\mathrm{HO}}=\sqrt{\frac{\hbar}{m \omega}}$ denotes the harmonic oscillator length, $L_{p}^{l}(\zeta)$ the generalized Laguerre polynomials and $C_{n, l}=\mathrm{l}_{\text {HO }}^{-1} \sqrt{\frac{2 p!}{(p+|l|)!}}$ a normalization constant, with $p=\frac{n-|l|}{2}$ the number of dark rings in the probability distribution $\left|\phi_{n, l}\right|^{2}$. These eigenfunctions are called LaguerreGauss modes.

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[^0]:    ${ }^{2}$ The line folds back if we insist using the periodicity of the structure and draw the full dispersion diagram in the first BZ.
    ${ }^{3}$ See Appendix A for more information about the used software.
    ${ }^{4}$ In general a wave with a wavelength $\lambda$ that obeys $m \lambda=2 a$, with $m \in \mathbb{N}$ will produce constructive reflections.
    These higher order reflections give rise to photonic bandgaps at higher energies.
    ${ }^{5}$ This can be rigorously shown using a variational theorem, see Joannopolous et al. [15].

[^1]:    ${ }^{6}$ This implies that $b^{i} \cdot b_{j}=2 \pi \delta_{j}^{i}$, where $\delta_{j}^{i}$ denotes the Kronecker delta function, i.e. the bases of the lattices are dual to one another.
    ${ }^{7}$ The $1^{\text {st }} \mathrm{BZ}$ is the Wigner-Seitz cell in reciprocal space.

[^2]:    ${ }^{8}$ This is the matrix containing the second-order partial derivatives with respect to the components of $\mathbf{k}$.
    ${ }^{9}$ We here also used the familiar relation between the energy of a photon and its (angular) frequency, which is given by $E=\hbar \omega$, with $\hbar$ the reduced Planck constant.

[^3]:    ${ }^{10}$ We have to assume here that this band is isolated from other bands in a sufficient large energy range containing the bottom energy. This assumption is valid in both the one-dimensional and two-dimensional PhCs that we consider in this manuscript.
    ${ }^{11}$ We factored out the time-dependency $e^{-i \omega t}$, as in Equation 2.3.
    ${ }^{12}$ For more information about these finite-difference time-domain (FDTD) simulations: see Appendix A.

[^4]:    ${ }^{13}$ This mask is a step function which equals 0 outside the selected region and is equal to 1 inside this region.

[^5]:    ${ }^{14}$ See Appendix A.

[^6]:    ${ }^{15}$ To check this, we of course had to run simulations employing higher resolutions as well.
    ${ }^{16}$ See Appendix B.

[^7]:    ${ }^{17}$ One can imagine that the larger $\sigma_{w}$ becomes, the worse the local density approximation holds. Another effect is that it gets harder to excite all the lower modes using one broad pulse. We have not extensively tested these limits. However this second issue seems to be the dominant effect and already appears in the case of perfectly quadratically chirped PhCs for larger values of $\eta$. In both cases, the mode frequencies can become very closely spaced and can have rather different Q -values, so that one of them is lost during the simulation.

[^8]:    ${ }^{18}$ In fact, from a radius of about 0.48 on, the second TE-band attains a lower minimum than the third TMband. This is not an issue here, since the lowest energy modes belonging to this band are sufficiently localized in the center of the crystal so that they do not extend into the outer region where the radii become of this order.

[^9]:    ${ }^{19}$ As in the case of the one-dimensional simulations, this high resolution was employed only to test whether a resolution of 32 sufficed.

[^10]:    ${ }^{20}$ All the $K$-points in the first BZ are assigned integers in a clock-wise manner, starting with 1 at the most left $K$-point.
    ${ }^{21}$ We have investigated the comparison up to $m=5$.

[^11]:    ${ }^{22}$ This, however, does not always work perfectly $[31,32]$.

[^12]:    ${ }^{24}$ There are higher order approximation schemes than the one described here, but this simple approach suffices here.

