List of corrections and examiners comments.

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Titel of thesis: Localization in Photonic Crystals

In the following the list of corrections and comments from all three examiners and the responses. The corrections and examiners comments are summarized for easier readability of the report. Each comment is followed by its response.

Comments from the first examiner:

Page 1: next to the last line, is linked => are linked
Fixed - As part of this chapter, we shed light on plasmons and their different types which are linked to the study carried out in a future chapter.

Page 1, line 21, "our" has to be deleted
Deleted.

Page 1. Last line the sentence could be rephrased, shortly explaining what plasmonic photonic crystals and photonic quasicrystals are.
We prefered to keep the introduction as short as possible and focus on highlighting the scope of the thesis at high level without delving into any technical and scientific details.

Page 2, line 1: components => topics
Fixed - The chapter serves as an introduction to the three main topics studied ....

Page 2, line 5: topic plasmonic => topic of plasmonic
Fixed - In chapter 5 we shift the attention to the topic of plasmonic photonic …

Page 2, line 6: a surface plasmon polaritons => surface plasmon polaritons.
Fixed - perturbation theory to calculate the impact of surface plasmon polaritons on the ….

Page 2, line 7: rephrase the sentence "Thus followed ..."
Fixed - A new paragraph was added:
The topic of optical localization is addressed in chapter 6, where we develop a scheme to compute the optical properties of photonic quasicrystals. Finally, in chapter 7 we present different schemes to identify localized states in optical systems. We provide two different examples where we study the states formed in the vicinity of defects in a regular photonic crystal, as well as the optical modes in a photonic quasicrystal.

Page 3, line 5: phenomenon => phenomena

Fixed - Regardless of the nature of the system, photons may interact with these electrons leading to a new set of phenomena.

Page 5, Sec 2.2, line 1: provide => provides

Fixed - The Drude–Lorentz model provides a framework for studying …

In the first line of Sec 2.2 and 2.2.2 the use of "between" (and "with" - "or", respectively) has to be revised.

Fixed - The Drude–Lorentz model provides a framework for studying the interaction between electrons and electromagnetic waves .....

And: The interface between a regular dielectric material (such as semiconductors or insulators) and a metal could witness the formation of evanescent surface charge density waves

The dotted lines in Fig. 2.1 are not so well distinguishable.

Figures were replaced.

Page 13, Acronyms should be expanded when using them for the first time in the text; e.g. MEEP (also see Appendix A)

Fixed - It is the preferred technique used by MIT Electromagnetic Equation Propagation (MEEP)

And: These scripts extended the functionalities of the standard packages of MIT Photonic Bands (MPB) for calculating the electromagnetic modes in periodic dielectric systems, and MIT Electromagnetic Equation Propagation (MEEP).

Page 15, line 17-18; the sentence has to be rephrased.

Fixed - For instance, 1D photonic crystals that consist of layers that are made of two different dielectric materials, will always have a band gap as long as the two layers have different dielectric functions with a suitable contrast.

Page 16, line 4 and 6 Fig. 3.1b => Fig. 3.1a

Fixed.

Page 16, line 8, Fig. 5.2a?

Fixed - now refers to the correct figure (3.1a)

Page 20, line 12-14: check the correctness of the sentence and/or give a better description

Fixed: The size and the density of the scatterers in addition to the wavelength of the wave in the media are essential in determining the type of the scattering; weak scattering occurs when the density is low and the scatterer–scatterer separation is large compared to the wavelength, and strong scattering occurs when the separation between the scatterers is small compared to the wavelength [45]

Page 24, line 16, form => from
Changed.

Page 26, line 8: it seems more correct to refer to Fig. 3.1a than Fig. 3.1b
Fixed: refers to the correct figure.

Page 27, explain what "conjugated-gradient-method" is or at least introduce a reference.

A new reference was added: This type of problems is better known as the Rayleigh-quotient, which can perfectly be solved using a preconditioned conjugate–gradient method [54]. The best description of this technique would be band-by-band minimization. It has been applied quite extensively in the study of electronic solids [55].

The references:
[54] P. Concus, G. H. Golub, and G. Meurant. Block preconditioning for the conjugate gradient method. SIAM Journal on Scientific and Statistical Computing, 6(1):220–252, 1985.

[55] M. C. Payne, M. P. Teter, D. C. Allan, T. A. Arias, and J. D. Joannopoulos. Iterative minimization techniques for ab initio total-energy calculations: molecular dynamics and conjugate gradients. Rev. Mod. Phys., 64:1045–1097, Oct 1992
Page 32, line 6: visa versa => vice versa
Changed.

Page 33, line 3: coved => covered
Changed.

Page 34, last sentence: it would be useful to have an indication of what is the experimental situation, namely what may be the practical changes in the dielectric constant.
That is discussed in page 35: It is also highlighted in page 35: For this to work, we have to ensure that for a given range of frequencies, the relative change in the dielectric constant ($\Delta\varepsilon/\varepsilon$) is less than 1%, such that Eq. 5.1 will give the main perturbative corrections. Under such conditions a first order perturbation theory is sufficient. However, larger fluctuations in the dielectric function might require higher order perturbation theories, or even iterative schemes.

Page 37, concerning the comment on the possible misleading generated by the Drude approach, it would be useful to introduce bibliographic references, if any, or - otherwise - underline the originality of the conclusion.
Added comments to the section to highlight the reason why the approach could be misleading: the Drude approach might be largely misleading in this aspect, since the overall change in the dielectric function at such frequencies can be quite remarkable, and the change in the band structure will be much larger.

It is also highlighted in page 35: See the previous comment.

Page 38, it would be useful to start with a definition of photonic quasicrystal and to explain the cut and project technique. "Inverse participation ratio" should be explained as well, and or a reference introduced.

Added a new paragraph: Quasiperiodic crystals (quasicrystals) are structures that demonstrate certain geometrical patterns but have no translational symmetry. The construction of quasicrystals involves non-trivial mathematical modelling, for example methods such as cut and project are used to build quasiperiodic structures, where a higher dimensional periodic lattice is sliced irrationally using a set hyperplanes and projected into a lower dimensional space under certain restrictions [63]. Such restrictions result quasiperiodic structures. In this work, the two–stage–projection method is employed to generate quasiperiodic lattices [64]. The two–stage–projection method is a special case of the cut and project scheme, but with the distinct advantage that only one-dimensional acceptance domains (i.e. intervals) are necessary in the first step, whereas the second projection step is usually trivial (i.e. choosing a layer), see Sec. 6.1.

Inverse participation ratio if found on page 38: Optical localization itself is determined using the analytical concept of an inverse participation ratio (IPR), which quantifies the number of states over which photons are distributed at a given frequency[4]

Page 38, line 10: state => stage

Changed.

Page 41 and 49: Braag => Bragg

Changed

Page 53: It would be useful to have a comment on the last sentence of sec 7.3, about the difference of an order of magnitude between the two computed results.

Added a comment: In contrast to the IPR presented in Fig. 6.4, we notice that the exponential decay is slower, which is attributed to the higher density of scatterers in the lattice. In turn, that leads to a smaller localization length ζ

Page 55, line 5-7: references are missing. The sentence on optical fibres to has to be corrected (and expanded). It is not the fibre which is surrounded by photonic crystals, it is the fibre core which is surrounded by a photonic crystal clad.

Fixed - The control over the properties of materials at all scales is a key in advancing new technologies. The development of sophisticated photonic technologies is a rich field of science due to many facts. For instance, in the field of solar cells, the control over the photons can help improve the performance of the cell in two different ways; filtering out photons with undesired frequencies [83] and enhance the absorption of photons within a certain range of frequencies [84]. Moreover, optical fibres can perform better in guiding beams of light when the fibre core is surrounded by carefully designed photonic crystals clad [85].

Page 56, the last sentence has to be rephrased since it is not very clear.

Rephrased - The perfectly matched layer is an imaginary material that is introduced in order to mimic the behaviour of the real system during a numerical simulation, and absorb all outgoing waves at the boundaries. A better approach should treat the boundaries as a genuine part of the system, which would improve the accuracy of the algorithm, reduce numerical errors and decouple the simulation from any artificial material.

Page 150: Ref [47] has to be completed (author name)
Fixed - E. Weinan. Principles of Multi-Scale Modeling. Cambridge University Press, Cambridge, 2011. But it is now [48]

Page 151: Ref [60] has to be completed (author name)
Fixed - L. Feng, X. P. Liu, Y. F. Tang, Y. F. Chen, J. Zi, S. N. Zhu, and Y. Y. Zhu. Tunable negative refraction in a two-dimensional active magneto-optical photonic crystal. Phys. Rev. B, 71(19):195106–195112, 2005

Appendix A: Expand acronyms MPB and MEEP. Also add references to packages websites.
See the comment above.

Comments from the second examiner:

Page 55: References do not appear
See the comments above.

Page 44 and 53: Explain the error bars in Fig 6.4 and Fig. 7.5
Explained in the caption of Fig. 6.4 - The decay of the inverse participation ratio as a function of the lattice size. The IPR values were extracted at frequencies between 0.59 – 0.649 (in units of $2\pi c/\alpha$) and averaged out. The error bars shown in the figure represent the deviation between each data point and the value obtained from the fitting.

Comments from the third examiner:

Page 3: nucleus uniformly charged with a negative elementary … (negative)?
Changed.

Page 7: When the E field is split into longitudinal and transverse components, it might be useful to include a brief discussion.
Added: To further analyse the fields associated with the plasmon oscillations, one can split E into a longitudinal and transverse component since plasmons are collective excitations, and hence one is dealing with matter waves, i.e. $E = E_l + E_t$.

The longitudinal component E l originates from the charge displacement, which causes the total charge distribution to deviate from its equilibrium value. That results in a new electric field source. Therefore $\nabla \times E_l = 0$ and $\nabla \cdot E_l = 0$. The plasmon equation becomes:

Page :7 Eq. 2.15, curl of E is 0 while the divergence is non zero. The opposite is true for E on page 8. Explain why.

See the comment above

Page 10: later assumption => latter assumption

Changed.

Page 10: explain more on extra momentum is needed to kick off an SPP.

Added notes: It is worth noting that SPPs cannot be directly excited by light due to their evanescent character. In fact light has to be coupled into an SPP using a prism or a surface grating since extra momentum is necessary to kick off an SPP and boost the modes frequency to match the light frequency [16].

Page 11: Eqs. 2.28, and 2.29 highlight the validity of the limits.

Reference cited: For the proper range of validity of these expressions with respect to the optical theorem see [19].

Page 12: Example on determining cross section using FDTD does not seem to contain any results. Also what are the parameters used in the simulation

The parameters are included in the caption of Fig. 2.1 and : This is demonstrated in the FDTD simulation presented in Fig. 2.1b, where a dielectric function was represented using the sum of Lorentzian resonances with parameters $\omega_1 = 0.065815$, $\gamma_1 = 0.31343$, $\sigma_1 = 7.9247$, $\omega_2 = 0.36142$, $\gamma_2 = 0.036456$, $\sigma_2 = 0.50133$, $\omega_3 = 0.66017$, $\gamma_3 = 0.0052426$, $\sigma_3 = 0.013329$, $\omega_4 = 0.73259$, $\gamma_4 = 0.07388$, $\sigma_4 = 0.82655$, ω_5 1.6365, $\gamma_5 = 0.19511$ and $\sigma_5 = 1.1133$. Further details and mathematical models for different geometries can be found in [19].

Page 13: Include a short summary.

Included: In this chapter we reviewed the aspects of light–matter interactions. We covered the frequency–dependent dielectric function and provided a derivation of the Drude–Lorentz model within the framework of Ehrenfest theorem. Furthermore, the interaction between electromagnetic waves and electrons was discussed in metallic systems where the electrons move freely around positively charged ions, which results in the bulk plasmon excitations.

At the interface between a metal and a dielectric material a new class of plasmons known as surface plasmon polaritons exist, which opens the door for a new set of applications that bridges the field of optics and electronics.

Moreover, the topic of localized surface plasmon resonances was covered in this chapter, where we finally presented a simple numerical simulation to compute the scattering as well as the absorption cross sections for a spherical silver nanoparticle. In the following chapter we lay the foundation of the numerical techniques used throughout this work.

Page 15: While the analogy between semiconductors/solids and PCs is drawn, comment on what is optical equivalent of the potential (atoms/molecules)

Included: In analogy to solids, dielectric elements like spheres or rods correspond to the atomic constituents of solids. Due to translational symmetry, the solution of Maxwell's equations yields photonic bands similar to those of the electronic systems.

Page 14: line 2 of Sec 3.1 the sentence is grammatically incorrect. Remove "arrangement"

Fixed.

Page 15: restrictions on the wave vector arise, why?

Highlighted: A key difference is the fact that 1D structures are
periodic along one axis (say z-axis for example). The 2D crystals, on the other hand, are periodic in a plane (say x-y plane in this case) which adds additional constraints on the wave vector k. To demonstrate those constraints, a 1D multilayer film would have a restriction on the k_z . In the 2D PCs the wave vectors parallel to the plane k are restricted to the Brillouin zone which is the periodicity direction, however, the k_z vector has no restrictions and modes along that axis propagate freely.

Page 16: There is a reference to Fig. 5.1, this is incorrect.

Fixed.

Page 16: Include the numerical details used to produce the band structure figures.

Details given: Fig. 3.1a depicts the transverse magnetic mode (TM) band structure for a two dimensional honeycomb lattice. The lattice points are populated with cylindrical objects of radius 0.2α, where α is the lattice constant. It is quite convenient to represent all bands in Fig. 3.1a in units of α, which stems from the fact that Maxwell's equations for systems with frequency–independent dielectric functions are scale–invariant [30]. The cylindrical objects on the lattice consist of a dielectric material of dielectric constant 13. The background medium is air (i.e. dielectric constant equal to 1).

Page 17: Sec 3.1.1 topic of great interest

Fixed.

Page 17: How were those values of lattice constant, sphere radius and refractive index obtained?

Values are obtained from the cited reference: In Fig. 3.3, we show the photonic band structure for an opal lattice with spheres of dielectric constant 3.35 and background material of dielectric 1.77. The spheres have a radius of 0.76 μm. In Fig. 3.3a the lattice constant is 1.88 μm, which corresponds to a chameleon with a relaxed skin. In Fig. 3.3b we present the band structure for lattice constant $\alpha = 2.55$ μm, which represent a chameleon with a stretched skin [33].

Page 18: How well do these calculated band structures in Fig 3.3 match the literature or how well do they explain recorded/observed chameleon colours?

The bands are similar to those published in ref [33].

Page 20: "a conducting system can turn into ..." rephrase the sentence.
Rephrased: Such a localized wave will decay exponentially over space. Consequently, a metallic system can turn into an insulator, because its conduction electrons become localized. This is not really covered by Bloch's theorem, which would still postulate extended states under the same conditions.
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Page 26: Add comments on the form of the operators A and B in Eq. 4.5 and the matrices that will be used to represent these.
Included: where A is the Hermitian operator on the left hand side of Eq. 4.4 and h represents the coefficient vectors (h 1 , h 2 , . . . h m). The matrix operator A is a result of the discretization of the momentum space used in the simulation. The matrix element A lm is given by Ψ † l A Ψ m and B lm is Ψ † l Ψ m. These products involve integration over the configuration space, in analogy to matrix elements in quantum mechanics [30].

Pages 35-36: For the sake of clarity it might be useful to include a schematic of the new plasmonic photonic crystal that is being simulated with perturbation approach.
Included: Fig. 5.1b

Why is the perturbation approach is used instead of other methods.
The aim is to develop new numerical techniques rather than using existing ones. The results in the chapter compare well to those in ref [37].

Page 36: More details on frequency matching.
Comments on page 35: To evaluate the effective frequency–dependant dielectric function, we increment the range of frequencies presented in the original band structure (Fig. 5.2a). Then, we iterate over all increments and determine the effective dielectric function for each frequency in the band structure that falls within the particular increment using Eq. 5.2.

Page 36-37: Some discussion on the breaking of the scale invariant nature of Maxwell's equations for plasmonic photonic crystals.
Included: It is important to mention that prior to the calculation of the effective dielectric function, the units of the frequencies have to be converted to rad/sec, which involve the lattice constant. Thus, the resulting solutions of Maxwell's equations are no longer scale-invariant, and the band structure will depend on the dimensions of a given plasmonic system. In other words, scale invariance requires frequency--independent dielectric constants, which may be justified for a typical photonic crystal, but not for plasmonic photonic crystals any more.

Page 37: are there any comments on the trend; how does the band gap change with lattice constant or with the ratio of metal/dielectric parameters?
The focus is developing new tools and verify that it works. The trends are not addressed since it is beyond the goal of the thesis. However, the tool does enable us to perform such studies.

Page 38: Might be useful to give a simple definition of photonic quasicrystal and inverse participation ratio.
See the comments from the first examiner.

Page 38: discuss some of the key concepts; why is aperiodic structure is more desirable? What are the considerations on boundaries in higher dimensional lattice? How does one choose the acceptance domain for two--staging--projection?
Details are given in the second paragraph of page 38: The unique properties of photonic quasicrystals such as a complete band gap at low index contrast [64, 65] are attributed to high structural symmetries [66]. The richness comes with the complexity of the mathematical modelling of quasicrystalline structures, in particular their relations to higher dimensional lattices.

Also a comments on two--stage--projection is found in page 38, the first paragraph:
The two–stage–projection method is a special case of the cut and project scheme, but with the distinct advantage that only one-dimensional acceptance domains (i.e. intervals) are necessary in the first step, whereas the second projection step is usually trivial (i.e. choosing a layer), see Sec. 6.1.

General comment: The boundary conditions are always absorbing boundary conditions since we use FDTD method. The details of the two--stage--projections can be found in [62].

Pages 41-43: As the size and the complexity increases, states start appearing at frequencies that correspond to band gaps. At what point in simulations (size of PQC) can a user stop and expect no further change. How does the results compare to experimentally fabricated PQC.
The details are addressed in the following chapter where we observe a smaller localization length for complex PQC. However, the change in the transmission depends on the geometry of the QC which was not investigated as part of the study. Please see the first examiner's comments on the chapter.

Are there any comments on the inverse problem where a lattice is mapped to obtain a certain frequency response?
No, that would require a different set of numerical tools with focus on optimization.

Pages 45-46: Any comments/insight into how this computation and results show trends that can be used to localise states in a desired manner. How does localization change with refractive index, PQC complexity, Is there dependence on the number of points used in the simulation?
As explained in pages 52 - 53, the results vary based on the geometry as well as the density of the points. However, we did not go into details of what influence the refractive index has on the localized states.