Exact Solutions in Lattice QED

Master Thesis

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September 2016

Die selbständige und eigenständige Anfertigung versichert an Eides statt.

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Unterschrift
Berlin,

Zusammenfassung

In dieser Masterarbeit wird eine vollständig orts- und zeit-aufgelöste Beschreibung von Quantenelektrodynamik (QED) vorgestellt. Der Ansatz basiert auf dem Hamiltonian im Ortsraum und ermöglicht, den gesamten (aber trunkierten) Fockraum der Theorie aufzubauen. Somit ist dieser Ansatz grundsätzlich nicht-perturbativ. Ableitung der diskretieierten Form des Hamiltonians erfolgt durch sehr allgemeinen Methoden, die sich leicht auf andere Quantentheorien übertragen lassen. Somit dient diese Arbeit auch der Vorstellung einer Diskretisierungs-Methodik. Um die Differentialoperatoren der Gleichungen zu approximieren, kommen zwei verschiedene Techniken zum Einsatz, die verglichen werden: Finite-Differenzen sowie eine Fourier-Methode. Dabei werden die Differentialoperatoren innerhalb der Fourier-Methode explizit aus der sogenannten diskreten Translationsgruppe mit Hilfe von gruppentheoretischen Techniken abgeleitet. Um das Framework zu testen, wurden Rechnungen in einem sehr simplen 1-Mode-2-Site Modell durchgeführt, die in allen untersuchten Beispielfällen gute Ergebnisse liefern. So kann zum Beispiel der Übergang zwischen QED und verschiedenen Grenzwerten anhand der Variationen des Energiespektrums dargestellt werden. Der nichtrelativistische, der starke Kopplungs- und der schwere Fermionen-Limes werden explizit gezeigt. Dabei erlaubt es das Modell, die verschiedenen Beiträge des Hamiltonians während diesen Übergängen separat zu betrachten und ihr Wechselspiel zu analysieren. Bei der Variation des Gitter-Abstandes zeigen sich Unterschiede zwischen beiden Diskretisierungsmethoden. Diese werden wichtig für kleine Abstände, was ein Zeichen für eine Verbindung zu Ultraviolett-Divergenzen ist. Schließlich erlaubt das Framework die explizite Untersuchung von Symmetrien und der Block-Struktur des symmetrisierten Hamiltonians. Das Potenzial des Modells für weitere Forschungsaktivitäten wird im Ausblick diskutiert.

Abstract

In this thesis, we present a fully space- and time-resolved numerical approach to quantum electrodynamics (QED). It approximates the Hamiltonian in real-space and is capable to build the complete (truncated) Fock space of the theory. It is by construction non-perturbative. We show the making of such a model and hence show a general discretization method for quantum field theories. We apply two different discretization methods, namely finite-differences and a Fourier method and compare them. In particular, the Fourier method is explicitly derived by the techniques of group theory. The discrete differential operator is deduced as a representation of the discrete translation group. We were able to make some proof-of-principle calculations in a very simple 1-mode-2-sites model that exhibit reasonable results in all analyzed cases. We visualize the transition between the full energy spectrum of QED and some limit cases: non-relativistic, the strong-coupling, and the heavy-Fermion limit. Our framework also allows for visualizing the interplay of the different contributions of the Hamiltonian within the transition. When we vary the spacing of the grid, we observe that both our discretization methods differ strongly for small spacings. This is probably connected to ultraviolet divergences and may be a starting point for the investigation of renormalization issues. Finally, we were able to analyze symmetries and the block-structure of the symmetrized Hamiltonian. The potential of the framework for further research is eventually discussed in the outlook.

Contents

1 Introduction

In this thesis, we present a fully space- and time-resolved numerical approach to quantum electrodynamics (QED). It approximates the Hamiltonian in real-space and is capable to build the complete (truncated) Fock space of the theory. In this sense, we construct exact solutions as mentioned in the title. In the following, we explain our motivations to develop such a model and give a short guideline through the work.

First of all, we want to emphasize that the techniques that are presented in this work are very general. They are applicable to any kind of quantum field theory and in this sense, this is more a technical work about discretization methods in quantum field theory and QED is an example of application. Consequently, our numerical studies are not about new topics, but they are rather proofs of principles. The main motivation behind the work was to investigate discretization from a physical point of view. Therefore, we try to look at the necessity of discretization not only as a mathematical but also as a physical problem. This leads to our main research question, which could be formulated as "what is the influence of the discretization on the ingredients of a physical theory: equations of motion, spinor-wave fields and symmetries."

Nevertheless, we needed to apply the method on a theory, and we choose quantum electrodynamics (QED). This is convenient for many reasons. QED is a fundamental quantum field theory, so there is no other theory that describes the electromagnetic interaction more precisely.[1] Consequently, it is a good starting point for such a fundamental analysis like ours. But at the same time QED is the one of the simplest quantum field theories with "only" Abelian gauge invariance U(1). We do not have to complicate the model by the treatment of non-commutating gauge-Bosons. Most important for our choice is probably the range of applicability of QED: the whole chemistry, molecular and atomic physics, solid state physics, plasma physics and even the physics of fluids and gases are "only" special cases of QED. It is a very complex theory and we reserve for its proper introduction to the whole first chapter 2.

Of course, in many situations it does not make sense to see, for example, chemistry as special case of QED. Most of the relativistic effects do not play a role, and often such limit cases are mathematically even more consistent and form a better point of view. But still there are relativistic effects that survive these limits. The most prominent example is undoubtedly the electron spin. It is an inherent property of fields on relativistic space-time, but not of the ones of Euclidean space. Hence, we need to include it manually in non-relativistic theories. Here we arrive again at our first research question: If symmetry is directly connected to such important properties like spin, what is the consequence for

[1] Although there are certain energy scales, where other interactions have a non-negligible influence on QED phenomena.

the corresponding symmetries of a discretized theory?

This of course is not new, and we know already a lot of effects that are due to the discretization. For example the Fermion-doubling problem.[2] What could we contribute with our method? Discretization is usually considered as a necessary tool to solve equations on the computer. Typically, all derivations are made as far as possible by means of the continuous theory and only the last step is the discretization, that then introduces some errors. Hence, another of our research questions is, "whether it matters, *on which level* the discretization takes place." Is for example the non-relativistic limit of a discrete QED-Hamiltonian the same as the discrete Pauli Hamiltonian?

In terms of the development of approximations to quantum theories, this can be very important. Especially mathematical rigorous proofs become substantially easier on a discrete lattice. For example, in time dependent density functional theory there is the very important theorem of v-representability that, so far, was only possible to proof rigorously on a lattice. As we cannot recapture density functional theory here to explain this example, we instead refer to the original publication by Farzanehpour and Tokatly [2012]. Instead, we want to point out the crucial point in the proof: the operators in the Hilbert space of the discretized theory become bounded, which simplifies the mathematical description enormously.

Additionally, our approach represents a conceptually new way to look at quantum electrodynamics. Typically, QED is solved perturbatively in scattering theory, so only in orders of the interaction strength. But the number of known effects that cannot be described so is constantly increasing with the experimental access to higher and higher energy scales. But even very basic physical settings like the ground state of a system are not describable by scattering theory. Our model with space- and (theoretically) time-resolution instead is per definition a non-perturbative theory. It is a Hamiltonian-based approach, which is not common in treating QED. We exploit the advantages of the canonical quantization procedure that typically is used for either non-relativistic or non-interacting theories. Furthermore, we introduce the field discretization by means of second quantization. This is shown in chapter 3.

In contrast to most of the other approaches, our model is defined on a real-space grid. In our opinion, this has two big advantages: First, probably most physicist would agree on the statement that real-space is most intuitive. Nevertheless most of quantum simulations are done in the reciprocal space and afterwards have to be Fourier-transformed for a good visualization. The tools of our approach could be applied to other theories to avoid such extra calculations.

Second, we use position space because we have the capabilities to do so. We actually can investigate generally the role of such representations of a quantum theory. On the

[2] See for example Frezzotti and Rossi [2004]

continuous level, the representations of any operator by any complete basis are equivalent. But in approximated and especially discretized theories, this is for sure not true anymore. One very interesting example is the photon position operator. Due to the vanishing photon mass, it is not possible to construct a meaningful operator, that measures the position of a photon [Bialynicki-Birula and Bialynicka-Birula, 2009]. This is the main argument why photons are usually represented in the reciprocal space. However, on a lattice this situation changes. Due to the inherent bandwidth-limitations, it is of course possible to say, whether a photon is on a certain grid point. Only when we want to resolve this point with arbitrary precision, the operator is not well-defined anymore.

Our last research question concerns the discretization method itself. In fact, there are various possibilities to discretize a differential equation and they have all different advantages and disadvantages. Consequently, there is for sure a difference between the techniques and the questions is, whether they differ crucially for any important parameter range. For quantum mechanical simulations, the most important techniques are finite-differences and Fourier transforms [Agarwal and O'Regan, 2008]. After showing in chapter 4 the application of finite-differences according to the most common method, we show its numerical results in chapter 5. We devote chapter 6 to a second method, which is a type of a Fourier method. Crucially, we derived the latter from a very untypical, but physically much more promising starting point. We tried to think about discretization in a more fundamental way and ended up at the symmetry interpretation of QEDSchwichtenberg [2015]. From this point of view, the most fundamental level of a relativistic quantum field theory is its symmetry. QED is a U(1) gauge theory on Minkowski-space that is defined by the Poincaré symmetry group. And indeed, all the ingredients of the equations of QED and even their form can be deduced from representation theory [Niederer and O'Raifeartaigh, 1974].[3] We derived the form of the discrete differential operators as representations of discrete symmetry operators. And it turned out, that this is equivalent to the Fourier method.

We eventually discuss the numerical results of the Fourier method and especially its comparison to the finite-differences method in chapter 7.

We complete the thesis with a conclusion in chapter 8 and in chapter 9, we give a little outlook on possible future continuations and new research topics.

[3] A quantum theory also needs further postulates, but the fundamental spinor-fields and their (classical) equations of motion are deducible from the symmetries.

2 Quantum Electrodynamics

Although this thesis offers rather general considerations about the discretization of quantum theories, the main focus in a physical sense is on Quantum Electrodynamics (QED), which we want to introduce in this chapter. We first give an overview about the theory, its mathematical classification and the problems of solving interacting quantum field theories like QED in section 2.1. Because of these problems, we have to discuss the properties of QED always under certain approximations.

We present a choice of such approximations in the second section (2.2). We introduce propagator theory as an example for a perturbative approach to QED in subsection 2.2.1. The corresponding solutions are derived in orders of the interaction strength, which is sufficient to describe a huge class of experiments. We mention the most important problems that have to be dealt with and discuss the limits of such approximations (subsection 2.2.2). Building on that, we shortly introduce lattice gauge theory in subsection 2.2.3. This is an important example of a non-perturbative approach. The last subsection (2.2.4) is about another non-perturbative approach, which is also a lattice theory but does not explicitly preserve gauge invariance. The focus here is on space- and time-resolved studies.

In the last section 2.3, we present the symmetries of QED. To do this properly, we introduce group theory in the first subsection 2.3.1. It is the mathematical framework to treat symmetries. Then we discuss Poincaré transformations (subsection 2.3.2) and gauge invariance (subsection 2.3.3) as the *defining symmetries* of QED.

2.1 Introduction to QED

Quantum electrodynamics describes the interaction between photons, electrons, and positrons on a full quantum mechanical level. Its corresponding phenomena are everywhere present on earth and even very important on astronomic scales. In fact, electromagnetism, optics, molecular physics, chemical reactions, solid-state physics, the physics of plasmas, and fluids can all be regarded as special cases of QED. Also in the theories of other interactions, QED plays an important role. It is more or less the only "measurement instrument" that man have because we see and feel on the basis of electric and magnetic forces [Białynicki-Birula et al., 2013]. Historically, QED was the first quantum field theory and it achieved firstly full consistence between the theory of special relativity and quantum mechanics. Consequently, there is much to say about it and this section only briefly summarizes the main concepts and the most important issues for subsequent parts. For a very intuitive introduction to QED, see the books of W. Greiner: Greiner and Reinhardt [2003] and Greiner et al. [2013], which also were often consulted to write this thesis. For a more exhaustive presentation of the topic, there is for example the book of Białynicki-Birula et al. [2013]. It explains the problems of the formulation of QED much better as

we could and so we want to conclude this introduction by summarizing this.

The problem in introducing QED is that there is no clear way to describe it, especially because QED is *not complete*. The postulates to define QED are still not proved to be consistent or unique. However, certain approximations of the theory allowed for the most precise theoretical predictions in the history of physics. Therefore, QED constitutes a "programme rather than a closed theory" [Białynicki-Birula et al., 2013]. It is based on two mathematically well-defined pillars. First, the quantum theory of electrons interacting with external classical electromagnetic fields and second, the theory of quantized Maxwell fields that interact with classical currents and charge densities. Combining both leads to so many difficulties, that there are many different formulations of QED. They all agree with respect to their numerical results but differ drastically in terms of mathematics. No theory could be derived with satisfactory mathematical rigor so far. One always needs somehow heuristic arguments. In this introduction, we present only the more or less unquestioned (mathematical) framework and the most important problems that arise in terms of the formulation of the full theory.

2.1.1 Definition of the Framework

In this subsection, we want to introduce the basis of quantum electrodynamics. It is built on the theory of Dirac-electrons coupled to external (classical) electromagnetic fields and the theory of Maxwell fields coupled to external (classical) charge currents. After introducing both of them shortly, we sketch how their combination in a proper mathematical framework leads to quantum electrodynamics. The main references are Greiner and Reinhardt [2003] and Białynicki-Birula et al. [2013]

Dirac formulated already in 1928 the quantum theory of relativistic electrons. The agreement between relativistic principles and quantum mechanics implies the introduction of Dirac-spinors ψ that describes not only electrons with their possible spin states but also positrons, their antiparticles. The free Dirac equation can be coupled in a mathematical consistent way to an external vector potential A^{μ}_{ext}[4]

$$(\mathbf{i}\hbar\gamma^{\mu}\partial_{\mu} - mc)\,\psi = e\gamma_{\mu}A^{\mu}_{ext}\psi. \tag{1}$$

Here $\mathbf{i}$ denotes the imaginary unit, $\hbar$ the Planck constant, e the electron charge, m the electron mass, c the velocity of light, and the γ^{μ} are the Dirac matrices that are defined by their algebra[5]

$$\gamma^{\mu}\gamma^{\nu} + \gamma^{\nu}\gamma^{\mu} = 2g^{\mu\nu},$$

[4] Minkowsi 4-vectors are denoted by a *greek* index. Their mathematical properties can be found in any standard textbook, for example in Gourgoulhon [2013].

[5] An explicit form is given in equation (61).

where $g^{\mu\nu} = \text{diag}(-1, 1, 1, 1)$ is the metric tensor in Minkowski space. $\bar{\psi}$ is the metric dual to ψ

$$\bar{\psi} = \psi^{+}\gamma^{0}. \tag{2}$$

We do not recall the general postulates of a quantum theory here; for an in-depth discussion of the theoretical framework see [Białynicki-Birula et al., 2013, ch.1, p.5]. We just mention that one can apply a quantum mechanical interpretation on ψ and its canonical momentum ψ^{+}, because the inner product $\psi^{+}\psi$ has the properties of a probability density. Specifically, the canonical formalism of the quantization of the free theory is summarized later in subsection 3.2.1.

The quantum theory of the Maxwell field is done by means of the quantization of the vector potential $\vec{A}$ with corresponding momentum $\partial_t \vec{A} = -\vec{E}$. They obey the inhomogeneous Maxwell equations

$$\partial_\mu F^{\mu\nu} = e j^{\nu}_{ext}, \tag{3}$$

with the electric field tensor

$$F^{\mu\nu} = \begin{pmatrix} 0 & -E_1/c & -E_2/c & -E_3/c \\ E_1/c & 0 & -B_3 & B_2 \\ E_2/c & B_3 & 0 & -B_1 \\ E_3/c & -B_2 & B_1 & 0 \end{pmatrix} \tag{4}$$

$$= \partial^\mu A^\nu - \partial^\nu A^\mu, \tag{5}$$

that is defined by the electric field and magnetic field vectors $\vec{E}, \vec{B}$ or by the four vector potential $A^\mu = (A^0, \vec{A})$, respectively. The latter definition implies the homogeneous Maxwell equations automatically. The inhomogeneity of (3) is formed by an the external four current $j^\mu_{ext} = (c\rho_{ext}, \vec{j}_{ext})$, that includes external charge densities ρ_{ext} and electric currents $\vec{j}_{ext}$. The quantum theory of Maxwell fields necessarily involves the vector potential and the related gauge invariance of (3). It is invariant under (local) gauge transformations of the form

$$A^\mu \to A'^\mu = A^\mu + \partial_t \xi(\vec{x}, t), \tag{6}$$

where $\xi(\vec{x}, t)$ is any differentiable function with the same domain as A^μ and in this sense makes the transformation local. This complicates the quantization process but methods where developed to also make the quantum field theory of free Maxwell fields coupled to external currents mathematically consistent. The canonical quantization procedure of the free theory is sketched in subsection 3.2.2.

Interestingly, gauge invariance turns out to be of major importance for the synthesis of Maxwell and Dirac theory. Also (1) exhibits the invariance under certain gauge transformations. They are of the type

$$\psi \to \psi' = e^{i\Theta}\psi, \tag{7}$$

where Θ is an arbitrary real number, which cannot vary in space or time, so this is a global gauge invariance. A modern way to derive the equations of QED is to generalize the global to a local gauge invariance to the Dirac field, so

$$\Theta \to \Theta(t, \vec{x}). \tag{8}$$

From this (differential geometric) point of view, QED is an Abelian gauge theory with symmetry group U(1). It describes spin-1/2 fields that - to be gauge invariant - necessarily interact through a gauge field which is the electromagnetic field. The resulting equations of motion look exactly as (1) and (3), when the external quantities are identified with the internal fields

$$A^{\mu}_{ext} \to A^{\mu}, \tag{9}$$

$$j^{\mu}_{ext} \to j^{\mu}_{Dirac} = \bar{\psi}\gamma^{\mu}\psi. \tag{10}$$

This "derivation" is summarized in subsection 2.3.3.

But the equations are not enough for a theory of quantum electrodynamics. It is necessary to make more postulates. Most important of those are the existence of a vacuum vector and the spectral condition, that together guarantee for a well-defined ground state. And requiring locality for field operators is necessary to guarantee causality. A complete list of requirements can be found in [Białynicki-Birula et al., 2013, sec. 19, p.311]. The latter postulates are of general nature and are true for every quantum field theory. This axiomatic approach was developed by A. Wightman and is more or less unquestioned. But these postulates are still not sufficient to determine the probabilities of physical processes. This is done by means of the *dynamical postulate*, which is the main difference between all the formulations of QED [Białynicki-Birula et al., 2013].

2.1.2 Solving QED

For QED like for every interacting quantum field theory there are no exact solutions known. Consequently, we always face approximations when we want to treat QED and we will introduce some important examples in the next section 2.2.

However, all approaches have to deal with major *inherent* difficulties. On the one hand, some of them arise from problems that are already present in the free quantum theories.

For the Maxwell field, the gauge invariance of the vector potential is not compatible with the canonical quantization formalism [Białynicki-Birula et al., 2013, sec. 8]. This can be cured in certain gauges, [6] but so the quantization of the Maxwell field is gauge dependent.[7] It is connected to the problem that photons have zero rest mass, and therefore, can have arbitrarily small energy in a quantum field theory. This is called *infrared catastrophe*.[8] Then, Dirac quantum theory already has a non-positive definite Hamiltonian, which is only physically interpretable if we perform light renormalization procedures and introduce antiparticles in some way. One method to do so is presented in subsection 3.2.1.

On the other hand, problems arise from the fusion of the two free theories. The already mentioned problem of the infrared catastrophe change its quality and is accompanied by an ultraviolet catastrophe[9] in full QED. The reason for both is the infinite amount of oscillators that is present in all quantum field theories. The infinities arising from that have to be treated by a renormalization scheme. The principal idea of renormalization is sketched in subsection 2.2.1.

2.2 Approaches to QED

In this section we present QED or better different aspects of QED by means of typical approximations. Propagator theory by Feynman and Stückelberg serves in the first subsection 2.2.1 as an example for the most common and most important approaches, that treat the interaction as a perturbation. It illustrates the involved processes well but cannot describe all regimes of QED. To describe for example bound states or space-time resolved experiments, other typically non-perturbative approaches are necessary.[10] We discuss the limits of propagator theory in subsection 2.2.2 and in subsection 2.2.3 and 2.2.4 we introduce two of the non-perturbative approaches.

2.2.1 The Classical Perturbative Approach: Propagator Theory

This subsection is about scattering theory, which is the most common approach to QED. It introduces perturbation theory and exemplary shows the most important properties of this regime. The content was mainly adopted from Białynicki-Birula et al. [2013]; Greiner and Reinhardt [2003]; Brown [2012].

Probably most famous among the approaches to QED is propagator theory. Propagator

[6] This is briefly discussed in subsection 3.2.2

[7] This is an important obstacle for the construction of a consistent quantum field theory formalism. See Strocchi [2004].

[8] It can be treated by analyzing the measuring process of observables. The interested reader is referred to [Białynicki-Birula et al., 2013, sec. 15].

[9] This also is known from classical electromagnetism, where the energy of a point particle diverges.

[10] There are also perturbative approaches that can describe bound-states of QED. We will not introduce them here but refer to Fried [2002].

theory was developed originally by Feynman and Stückelberg [11] and gives a comparatively intuitive picture of the involved processes. It is formulated with boundary conditions that are typically realized in scattering experiments and that are crucial for the description. Specifically, given a state $|\psi_i\rangle$ that shall describe a wave-packet that was prepared so long ago that there are no interferences present to a second somehow scattered wave-packet $|\psi_f\rangle$ that is measured long time after the scattering process, then the overlap of both states and hence all information on the scattering process can be expressed by the so-called S-Matrix that is the time-evolution operator from $-\infty$ to ∞

$$\langle\psi_i \,|\, \psi(t\to\infty)\rangle = \langle\psi_i \,|\, S \,|\, \psi_f\rangle = \langle\psi_i \,|\, U(-\infty,\infty) \,|\, \psi_f\rangle\,. \tag{11}$$

In the interaction picture[12] with time-dependent interaction operator $V(t)$, one can derive a formal expression for the S-Matrix

$$S = U(-\infty,\infty) = T\exp\left(-\mathbf{i}\int_{-\infty}^{\infty} V(t)\mathrm{d}t\right), \tag{12}$$

where T denotes the time-ordering operator. The S-Matrix is obviously very convenient as the starting point for perturbation theory in orders of the interaction strength. Most of the perturbative approaches treat only the S-Matrix.[13] The series in orders of $V(t)$ is formally very easily derived by the expansion of the exponential

$$S = \mathbb{1} - \mathbf{i}\int_{-\infty}^{\infty} V(t_1)\mathrm{d}t_1 + \frac{(-\mathbf{i})^2}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} T[V(t_1)V(t_2)]\mathrm{d}t_1\mathrm{d}t_2 + \ldots \tag{13}$$

This is called Dyson series and can be seen as the desired perturbation series if $V(t)$ is small with regard to the free Hamiltonian. In QED, the interaction term is

$$V = e\, j^\mu A_\mu = e\,\bar\psi\gamma^\mu\psi\, A_\mu. \tag{14}$$

When we integrate this properly in (13), the small parameter is given by e^2 or in dimensionless form by the fine structure constant $\alpha \approx 1/137$. The smallness of α is the reason for the enormous successes of the theory. Although there are strong arguments that (13) does not converge, there are regimes of QED, that are unaffected by such higher order divergences. This is discussed in the next subsection 2.2.2.

[11] The original publication by Feynman was [Feynman, 1949].

[12] The interaction picture takes advantages from the fact that free theories are possible to be solved exactly by use of the eigen-representation of the kinetic operators. Let $H(t) = H_0 + V(t)$ be the Hamiltonian of the system that may be split into the free part H_0 and the interaction $V(t)$. Hence, time evolution can also be split into a free part that is carried by the operators and the interaction part that is carried by the state vectors. Hence it can be regarded as an intermediate representation between the Heisenberg and the Schrödinger picture.

[13] I. Birula for example formulates QED actually on the basis of the S-Matrix in [Bialynicki-Birula and Bialynicka-Birula, 2009, ch. 6]. Hence, the S-Matrix is the dynamical postulate in contrast to the Heisenberg equation with a Hamiltonian in the canonical procedure.

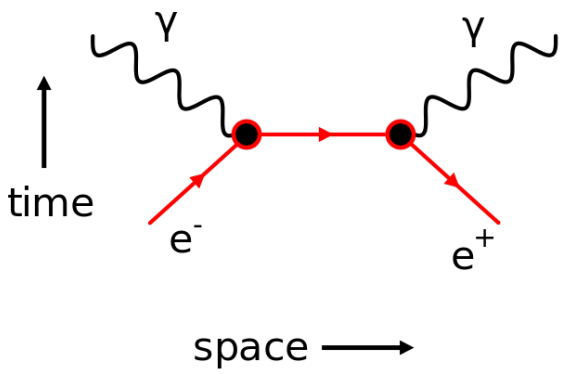

FIG. 1: The Feynman diagram of an electron-positron annihilation experiment is shown. The red solid lines represent electron and positron propagators S_F. The curved lines are instead photon propagators D_F. The black dots are called vertices and the total number of vertices counts the elementary interactions. It also denotes to order of the perturbation series that exhibits this graph. This figure represents one integral of the second term in (13).

With the aid of Wick's Theorem[14] we can apply the Feynman diagram method on the Dyson series. It introduces a direct link between the terms of (13) and graphical representations, that are called Feynman diagrams. An example of such a diagram is depicted in figure 1. Wick's theorem brings the terms of (13) in a form, that consists of three ingredients:

1. Dirac-propagators $S_F(x-y)$[15], which are the Green's functions of the free Dirac equation. In quantum field theory, $S_F(x-y)$ can be expressed as

$$\mathbf{i}S_{F\alpha\beta}(x-y) = \left\langle 0 \left| T(\psi_\alpha(x)\bar{\psi}_\beta(y)) \right| 0 \right\rangle . \tag{15}$$

   They are represented by solid (red) lines with starting point x and endpoint y in the diagram in figure 1. Then

2. photon propagators $D_{F\mu\nu}(x-y)$, that are instead the Green's functions of free Maxwell equations. Hence their explicit form is gauge dependent but the abstract definition of the quantum mechanical Green's function is still applicable

$$\mathbf{i}D_{F\mu\nu}(x-y) = \langle 0 \,|\, T(A_\mu(x)A_\nu(y)) \,|\, 0 \rangle . \tag{16}$$

   They are represented by wiggly lines in 1. Finally,

3. vertices, that represent the order of perturbation and hence the number of integration variables and the number of elementary interactions. They add a factor $\mathbf{i}e\gamma^\mu$

[14] This is a method to find the implications of the time-ordering operator for arbitrarily large terms of such a perturbation series [Greiner and Reinhardt, 2003].

[15] The index F refers to the developer of the concept: R. Feynman. With $x \equiv x^\mu$ and $z \equiv z^\mu$, we denote space-time coordinates. We spare the index $^\mu$ in this subsection.

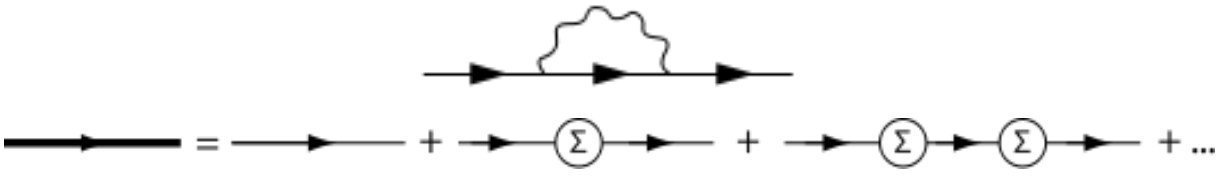

FIG. 2: A loop diagram for a Dirac propagator S_F is shown in the upper picture. It contributes to the self-energy Σ of the respective particle. In the lower picture diagram of the dressed propagator S'_F is shown. Infinitely many loop diagrams contribute to its self-energy. Source: Wikipedia.

to the integral and they are represented as dots in figure 1.

Practically one can interpret such a perturbative approach as follows: the zeroth order describes free plane waves, the first order adds one scattering event (one vertex in a Feynman diagram), the second order allows for one and two interactions and so on.

Within propagator theory, the emergence of the already mentioned infinities can be visualized easily and it also provides a framework to deal with them. One origin of infinites is visible in the propagators themselves. One can introduce the *dressed Dirac propagator* S'_F, that is defined as the sum over all possible diagrams that connect two vertices. It is an infinite sum because there can be infinitely many so-called loop diagrams in between the points. The diagrams for a loop and the dressed propagator are depicted in figure 2. For photons one can make the same considerations and also find a self-energy that is also called vacuum-polarization. Self-energies in QED can be shown in perturbative theories to diverge linearly with high energies. These infinities are due to ultraviolet divergences and are a general feature of quantum field theories.[16] There are so many high energy modes that every sum over these diverges. The second reason for infinities can be found in the vertices, which similarly can be dressed with loop diagrams. This is qualitatively different to the self-energy. The divergence is logarithmic with higher energies.

Additionally, there are infrared divergences present that originate from the photons having rest-mass zero. The propagator diverges for a vanishing wave-vector. This is in contrast to the Dirac field, which due to is mass m exhibits a finite energy mc^2 for zero wave-vector. In different words, there are not only infinitely many photons with very high but also with very small energies. Hence, the integral with domain border $k = 0$ over any product of photon propagators must diverge.

Notably, divergences can at least in a perturbative sense be rigorously removed through the so-called *renormalization program*. It is based on the observation that on certain energy scales, QED performs very well in predictions. [17] But as we saw, for much smaller or higher energies, it exhibits divergences. Hence, the main idea of renormalization is

[16] Although the exact form of divergence cannot be deduced in most of the non-perturbative approximations.

[17] Many physicists would argue that QED is the best existing physical theory, because it allowed for

to rescale some quantities of the theory in a way that they counter the divergences. For QED, we argue that this must be possible, because of its good performance on the medium scales. Luckily, there are exactly enough parameters in the theory to counter all the occurring infinities. The renormalization program is applicable. The parameters are the electron mass m_e and the coupling constant e, as well as the Dirac and Maxwell field-normalization factors. Of course, we need a physical interpretation for these energy-dependent "constants." One could argue that physical objects can never be measured under exclusion of the interaction to their environment. In an experiment, we just can determine something like the *experimental value* of the electron charge. But the electron charge that appears in the equations instead, would have the *bare value*. In the propagator picture, the free propagator would be defined with the bare constants, and the dressed operator would exhibit the corrected experimental value. Hence, the infinities of, for example, the self-energy corrections are countered due to altering bare constants.

The details of the renormalization program can be found in Bialynicki-Birula and Bialynicka-Birula [2009] and Brown [2012].

2.2.2 The Limits of S-Matrix Theory

In this chapter we shortly want to classify the limits of all the perturbative methods that involve the S-Matrix on a phenomenological basis.[18] The objective is to collect the reasons that led to developing other approximations.

First of all, as we already mentioned, the Dyson series does very probably *not converge*. It was Dyson himself, who argued that the radius of convergence of a perturbation series in the electric charge must be zero, because a negative coupling constant would "reverse" the electromagnetic forces, and hence create a completely different theory. Formally, this is incompatible with a well-defined vacuum [Białynicki-Birula et al., 2013]. These arguments set general limits to the perturbative approach, although it is not always clear, on which scales they appear exactly.

But for some physical settings, this is actually very clear. The *ground state* of a system for example would necessarily involve all orders of perturbation theory and hence is definitively part of the non-perturbative regime.

Additionally, it is not possible to calculate the ground state by means of S-matrix theory, because the required *boundary conditions* of uncorrelated plane waves for $t \to \pm\infty$ cannot be fulfilled. There are also other examples for the insufficiency of the S-Matrix. The solutions of the Coulomb problem for example never converge to a plane wave. Rohrlich

the most precise predictions, that ever have been done. The value of the magnetic moment of an electron for example can be calculated and measured on the 13th decimal place [Odom et al., 2006].

[18] There are also other perturbative expansions for QED like generalized Green's functions formalisms that overcome some of the insufficiencies of the S-Matrix theory. We will not recapture them here. See for example Fried [2002].

[1980] discussed such problems.

Another very important shortcoming of the S-Matrix approach is that we loose all information about the space- and time-resolved dynamics. For example, the actual absorption and emission processes of photons cannot be understood [Wagner et al., 2011]. We present in subsection 2.2.4 an approach that is non-perturbative and is capable to provide space- and time-resolution.

Finally, we want to emphasize again that the perturbation theory is only applicable on QED because of the small coupling constant. In other quantum field theories from the standard model, this is not true anymore and so there is no chance to solve them perturbatively. The most successful tool to calculate typical problems of for example quantum chromodynamics (QCD) is *lattice gauge theory*, which will be introduced in the next subsection (2.2.3).

2.2.3 Lattice Gauge Theory

This subsection is about lattice gauge theory, which is a very important tool to describe more complicated gauge theories than QED. Although its techniques are of minor interest for our purposes, it is introduced because it is the most successful approach to quantum field theories on a lattice.

Lattice gauge theory was developed for quantum chromodynamics (QCD), the quantum field theory of strong interaction [Wilson, 1974]. QCD is a gauge theory with the gauge group U(3). The coupling between the 12 dimensional Fermionionic spinor and the 8 gauge fields of QCD is in dimensionless form of the order of 1. Hence, we cannot approach it within a perturbation theory like the propagator theory of QED. Moreover the treatment of its 8 gauge Bosons is much more complicated than that of the photon in QED. Instead, one could try to develop a theory that describes the dynamics of a quantum field theory on a space-time grid, as it is common in non-relativistic theories. The problem here is that a lattice cannot approximate a flat space and the geometric structure of the gauge symmetry[19] at the same time [Wilson, 1974]. If gauge symmetry is not treated properly, its continuum limit is wrong. And the gauge fields on the lattice are not well described. Lattice gauge theory overcomes these difficulties by the introduction of a modified action. In this way, gauge invariance can be preserved in a way, that the discrete gauge fields approach their continuum limit continuously. The first formulation of such a theory was due to Wilson [1974].

However, as this work is about Lattice QED, that does "only" exhibit U(1) symmetry, we do not have to struggle with the problems related to gauge invariance. Therefore, we spare the introduction of the theory apparatus and for example refer to Lin and Meyer

[19] This structure is called a fibre-bundle and can be viewed as space of all possible coordinate changes, which are determined by the gauge symmetry group.

[2014].

2.2.4 Space- and Time-Resolved QED

This last subsection of approaches to QED sketches another lattice field theory, that the group of R. Grobe recently started to develop [Wagner et al., 2011]. It is built to study space- and time-resolved processes. Although Grobe's group makes use of different numerical techniques, their approach is very comparable to the one presented here, and so it delivers some techniques that we can adopt in the future.

The goal of this approach is to investigate elementary effects like photon absorption and emission on high energy scales. This involves strong relativistic effects and makes a full QED treatment necessary. This goal is still kind of far but they could already obtain some good results for model theories [Wagner et al., 2011]. Their model is formulated in a Hamiltonian formalism in momentum space. It is discretized by imposing periodic box boundary conditions and truncating the Bosonic space. As the dimension of the Fock space in relativistic theories grows extremely fast with the number of grid points, this approach is limited to very small systems.

So far, Grobe's group analyzed some aspects of the interaction between Fermionions that is mediated through Bosons and virtual Bosons. Recently, they could present a renormalization scheme that can be applied to a discretized Hamiltonian Wagner et al. [2013]. They found logarithmic divergences in the spectrum of the Hamiltonian.

2.3 Symmetries of QED

Eventually, we want to introduce an aspect of QED, that has rather different qualities. The topic of this section is to look at QED from the point of view of its (defining) symmetries.

It was already mentioned that QED was historically the first theory that unified special relativity and quantum mechanics. Within this process the theory of special relativity was proven to be much more important than just in changing some velocity laws. In fact, one may be allowed to say that the development of special and later general relativity introduced a whole new interpretation and view on physics.

One of these important changes emerged due to a deeper understanding of symmetries. Of course, symmetries have been regarded important already at the beginning of classical mechanics by Newton and Leibniz, but probably there is no doubt that the derivation of the famous theorem by Emmy Noether [Noether, 1918] changed the perspective on symmetries fundamentally: Symmetries induce conservation laws, which proved to be among the most important tools to solve the complicated differential equations that describe

physical systems. Consequently, symmetries became more and more the main player for the investigation of a physical system instead of forces and fields: While in Newtonian physics a problem was solved by finding the correct force, plugging it into the Newtonian equation and adopting the latter to the physical setting,[20] physicist started in the last century to think first about the symmetries of the systems and then to construct the theory according to that. The theory of special relativity, for example, does not need something like Newtonian laws at all, but just the postulates of momentum and angular momentum invariance.[21]

Hence, it may not be a coincidence that Noether's theorem was discovered in 1918, in the pioneer years of the theories of relativity. General relativity taught us finally that all our basic physical concepts like energy or momentum do only make sense if there is a corresponding symmetry according to Noether's theorem: Energy does not exist without time translation invariance.[22] Today's physicists started to describe all dynamics as symmetry transformations of certain tensors that somehow contain the information about physical objects. But even all these possible physical objects can be deduced from some assumed fundamental symmetries of the universe, so that there are just some free parameters left to define whether a theory describes a (free) electron or a (free) neutrino.[23] In the framework of the Standard Model one can further deduce all interactions from a second type of symmetry which is called gauge invariance. Steven Weinberg once formulated it like this: "The universe is an enormous direct product of representations of symmetry groups." Gallian [2016]

Of course all this is mainly a question of interpretation, but when we developed our approach, this interpretation proved to be a very good starting point. And so we want to introduce it properly in this section. We first recapitulate the mathematical tool to study symmetries, which is group theory (subsection 2.3.1). Then we introduce the Poincaré group, which is the symmetry group of Minkowski space, the proper mathematical space of relativistic space-time (subsection 2.3.2). We summarize its elements and group structure and sketch how representation theory can be used to characterize all the spinor-fields that can be realized in Minkowski space. It is even possible to deduce the covariant wave equations for these (free) spinor fields (so including Maxwell and Dirac equations), which we do not show explicitly but refer to sources. We conclude with a subsection on gauge

[20] This turned out to be so complicated that a complete new theory had to be developed: Lagrangian mechanics.

[21] This approach is very accurately developed in, for example, Gourgoulhon [2013].

[22] This means that we always need a certain observer system that exhibits such invariance and hence defines energy.

[23] This is meant in terms of the respective equations of motion. Of course, equations and their solutions have to be interpreted according to experiments and generally, there are many conceptual assumptions behind physical theories that cannot be derived from any higher principle. Nevertheless, the equations of motion of a theory are a very important if not the most important tool for a physicist and the derivation of equations just by means of symmetries was surely an important step in the development of physics.

invariance, which is crucial for the formulation of QED (2.3.3). We demonstrate how the QED Lagrangian can be deduced from imposing local gauge invariance on the Dirac equation, which can be deduced from Poincaré symmetry. In this sense, QED is defined by its symmetries.

2.3.1 Group Theory

We now introduce the main ingredient to study symmetries, which is group theory. The contents of the chapter are mainly taken from Wagner [1998]; Gourgoulhon [2013]; Greiner [2000]; Lyubarskii [2013].

Fundamental symmetries in physical contexts have the great advantage that they can be regarded mathematically as Lie groups. They have been investigated since the late 1880th and are very well understood today which may be the reason for the great success of symmetry considerations in physics. The crucial property for treating a certain symmetry transformation in terms of group theory is that it is *linear*, which means it admits a (faithful) representation as linear transformations on a vector space. The typical argument is that space-time must be homogeneous, which means that no point is special in relation to any other point, because why should it? Then one can proof that the transformations that connect the points have to be linear[24]. This is not true anymore in general relativity where every type of energy changes space-time and hence destroys its homogeneity. One could say that then at least the vacuum should be homogeneous, but as we know from quantum mechanics that there are vacuum fluctuations, even this argument does not apply anymore. Nevertheless one could at least assume approximative homogeneity of space-time and hence apply group theory on its symmetries, which still turns out to be very successful.

Let us start with the definition of a group, following Wagner [1998]. A group G is a set of elements together with a group operation (we generally call it composition) that fulfill

1. composition of the group elements results again in a group element:
   $a, b \in G \Rightarrow c = ab \in G$,
2. associative law: $a(bc) = (ab)c$,
3. existence of the identity $e \in G$: $re = er = r \quad \forall r \in G$,
4. existence of the inverse r^{-1} to r:
   $\forall r \in G \; \exists r^{-1} \in G \quad \text{with} \quad rr^{-1} = r^{-1}r = e$,
5. groups that additionally fulfill the commutation law
   $ab = ba \quad \forall a, b \in G$
   are called *Abelian*.

[24] A good discussion can be found in Stackexchange-Physics [2011]

The key part with respect to symmetries is the so-called representation theory. The representation T of a group is defined as a homomorphic map from the group G on a linear space L (which can always be identified with the space of matrices M) that „conserves“ the product:

$$T(g_1 g_2) = T(g_1)T(g_2) \quad \forall g_1, g_2 \in G. \tag{17}$$

Of course there is an infinite amount of representations of one group but it is actually possible to find them all up to so-called *equivalence*, which demonstrates the strength of the formalism. Two representations T and T' are equivalent if:

$$\exists M \in L: \quad T'(g) = M^{-1}T(g)M \quad \forall g \in G. \tag{18}$$

The next step in finding all the representations is the important theorem that a representation can always be decomposed in its *irreducible* representations T^i

$$T = T^1 \oplus T^2 \oplus \cdots \tag{19}$$

where the T^i are *also* representations of G and there is no further such decomposition for them. This can be interpreted as a *blockdiagonalization* in the matrix picture:

$$T(g) = \begin{pmatrix} T^1(g) & 0 & \cdots \\ 0 & T^2(g) & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}. \tag{20}$$

Every block contains one irreducible representation of the whole group. When we have found all these possible blocks, we have found all representations up to equivalence.

We want to apply these properties to a certain example of groups, the so-called Lie groups. A group G is called Lie-Group if

1. it is *continuous*, so every element $g \in G$ can be regarded as a continuous function,

2. every $g \in G$ has a *finite* amount of parameters $\{\alpha_i \in \mathbb{R}\}$ that describe it completely. The minimal number of such parameters is called the *dimension* d of the Lie-Group, and

3. the elements are differentiable with respect to the parameters.

Another way to say this, is that a Lie group G is isomorphic to a manifold M with dimension d. Because of this, we can describe the local structure of G through a so-called *Lie-Algebra* G_A whose underlying vector space is the *tangent space* of M. A basis is given

by the d so-called *infinitesimal* operators

$$I_j^T = \left.\frac{\partial T(\vec{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_d))}{\partial \alpha_j}\right|_{\vec{\alpha}=\vec{0}}, \tag{21}$$

where the point $\vec{\alpha} = \vec{0}$ coincides with the identity T(E). Hence, the Lie-Algebra G_A is the linear span of the set of infinitesimal operators $I_j\,(j = 1, 2, \ldots, d)$ together with their algebraic structure. For the matrix representation it can be formulated through the commutation relations between the elements

$$I_j I_k - I_k I_j \equiv [I_j, I_k] = \sum_{i=1}^{m} C_{ijk} I_i, \tag{22}$$

with the *structure constants* C_{ijk}, that are independent of the representation T. The crucial point is that there is a surjective map between any Lie-group and its Lie-Algebra. But there is always one Lie-group to every Lie-Algebra that maps bijective to it, which is *simply connected*.[25] It is called the *covering group* G_{cover} of G_A. In other words, there is a set of Lie-groups $\mathcal{G} = \{G\}_{G_A}$ which all share the same Lie-Algebra G_A (so the same local structure) and there is a map from one special element $G_{cover} \in \mathcal{G}$ to every other element of $\mathcal{G}$ but not back. G_{cover} "covers" the other elements. All this is because of the manifold structure of a Lie group: every finite group action can be composed by a repeated application of the infinitesimal operator. Schwichtenberg [2015]

Mathematically, the map between G_A and G has in most cases a very simple form: it is the *exponential map*.[26] One representation $T(g)$ of any element $g \in G$ is given by

$$T(g) = e^{-\mathrm{i}H}, \quad H = \sum \alpha_i I_i. \tag{23}$$

with a certain set of $\{\alpha_i\}$. This is why the I_i are also called generators: I_i "generates" the transformation that is determined by the parameter α_i ("in the direction of I_i").

In terms of quantum mechanics we describe symmetry transformations as operators that preserve the inner product, so that expectation values for example are invariant under such transformations. Therefore, we look for a representation $T_{\mathcal{H}}$ in a Hilbert space $\mathcal{H}$ (with inner product $\langle \cdot \,|\, \cdot \rangle$) that obeys

$$\langle T_{\mathcal{H}} f \,|\, T_{\mathcal{H}} g \rangle = \langle f \,|\, g \rangle \; \forall f, g \in \mathcal{H}. \tag{24}$$

Wigner and Bargmann could prove[27] that such representations are either unitary or anti-

[25] This means that any closed curve on its corresponding manifold can be shrunk smoothly to a point.

[26] To be precise, it is only true for groups with matrix representations, so also for all examples treated in this work. Nevertheless there is a slightly more general definition that is even true for *all* groups. See fore example [Gourgoulhon, 2013, sec. 7.4.1]

[27] This can be found for example here [Thaller, 2010, Th. 2.7].

unitary.[28] Hence, we can always choose in the following those among all equivalent representations that are (anti-)unitary.

With the help of the Lie-Algebra we have a very good access to the group and can investigate any compositions or functions of the generators. Very interesting among those are certain operators C that have a vanishing Lie-bracket with all of the infinitesimal operators

$$[C, I_j] = 0 \quad \forall\, j. \tag{25}$$

These are called *Casimir* operators and they represent something like the "fundamental symmetries of a symmetry group." One of the most important properties of a Casimir operator is that it can be used to construct the irreducible representation. This is because if C is invariant under the action of any element $g \in G$, then all eigenfunctions of C Ψ^l with

$$C\Psi^l = l\Psi^l$$

also must be invariant under G in the sense, that they keep their eigenvalue

$$C'\Psi'^l = l\Psi'^l,$$

where the ' denotes that any $g \in G$ acted on the respective object. Then the complete set of linear independent eigenfunctions Ψ^l_m, $m = 1, 2, ..., d_l$ (with degeneracy d_l) build a basis for the representations with dimension d_l of the group. If this symmetry group is the highest possible (that means that there is no group $G' \supset G$ that leaves O also invariant), the representation can be proven to be irreducible.[29].

Having introduced the mathematical apparatus, there is still the question of its connection to physics. This lies in the symmetry interpretation of a group. Space-time can actually be defined through its symmetries. In our case of QED (but also for the whole standard model) space-time is the Minkowski space M^4 which is defined through the Poincaré symmetry group. Through representation theory this induces a vector bundle V: the set of vector spaces for every irreducible representation. Then physical states (of a classical field theory) are introduced as sections of M^4 that are characterized by the eigenvalues of the respective Casimir operators. These correspond to the mass and the spin of the field, which we know from experiments. For every such section, a wave equation that is covariant with respect to G can be deduced. In this sense, Maxwell equations or the Dirac

[28] A unitary operator U is linear and obeys 24, whereas an anti-unitary operator A is instead anti-linear, so $A(a\vec{x} + b\vec{y}) = a^* A(\vec{x}) + b^* A(\vec{y})$.

[29] But even if it is not the highest possible symmetry group, it nevertheless can induce irreducible representation in certain cases. See Wagner [1998]

equation are just representations of the Poincaré group. [30]

2.3.2 Poincaré Transformations

Basing on the previous subsection, we are able to properly introduce the fundamental symmetries of the theory of special relativity, namely Poincaré transformations. We follow the presentations in Gourgoulhon [2013] and Greiner [2000].

Poincaré transformations are defined through the concept of a so-called inertial observer, which physically means that the description of a certain experiment is made in coordinate frames, that have vanishing acceleration in the Newtonian sense. The proper mathematical space that exhibits such frames is an *affine* (flat) space $\mathcal{E}$ over $\mathbb{R}$. Experience tells us that it must have 4 dimensions, 3 for space and 1 for time. Affine spaces are manifolds and hence, they can be mapped at every point to a vector space E that for a 4D manifold is isomorphic to $\mathbb{R}^4$. The special property of a flat space is that one coordinate frame is enough to describe every point in $\mathcal{E}$. Inertial observers now refer to the special coordinate frames which "see" the same so-called line element $\mathrm{d}s$. Mathematically it is defined in *any* coordinate system $\{x^\mu\}$ of $\mathbb{R}^4$ with the aid of the metric tensor[31]

$$\mathrm{d}s^2 = g_{\mu\nu}\mathrm{d}x^\mu \mathrm{d}x^\nu. \tag{26}$$

If such a frame is inertial, the metric tensor has the simple diagonal form

$$g_{\mu\nu} \overset{\text{inertial}}{=} \eta_{\mu\nu} \equiv \mathrm{diag}(-1,1,1,1), \tag{27}$$

$$\rightarrow \quad \mathrm{d}s^2 \overset{\text{inertial}}{=} -(\mathrm{d}x^0)^2 + (\mathrm{d}x^1)^2 + (\mathrm{d}x^2)^2 + (\mathrm{d}x^3)^2 \equiv -(c\mathrm{d}t)^2 + \mathrm{d}\vec{x}^2, \tag{28}$$

where in the last part the time and space components[32] were already separated. In 1905 this was derived by Einstein in his famous work by postulating the invariance of the speed of light c, which enters the above definition to give the time axis the same unit like the three space axes. We see the invariance of a velocity in the definition easily because of the different sign of space and time

$$\frac{\mathrm{d}s^2}{\mathrm{d}t^2} = \frac{\mathrm{d}\vec{x}^2}{\mathrm{d}t^2} - c^2 = const.$$

$\eta_{\mu\nu}$ is called Minkowski metric and it defines the basic geometric structure of $\mathcal{E}$, the inner

[30] For a general derivation of *all* Poincaré covariant wave equations see Niederer and O'Raifeartaigh [1974].

[31] Note that this is mathematically not a metric.

[32] To distinguish between four-vectors and purely spatial three-vectors, the latter are denoted with an arrow.

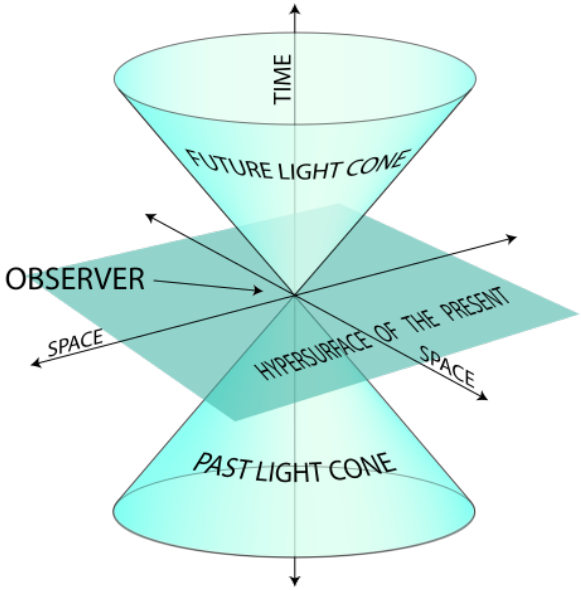

FIG. 3: The light cone for 2+1 D Minkowski space is depicted. It describes the geometric properties of the Minkowski space M^4: From any point in $p \in M^4$ one of its two cones shows the future and the other the past time direction. Inside the cones lie all possible time-like distances, so all possible trajectories of a massive object that cross p. Outside the cones lie all space-like separations, which physically means that there is no possibility to exchange any information. The cone itself is defined as the set of all light-like vectors, so all possible trajectories of a light signal. Image: Wikipedia.

product between two vectors $a^\mu, b^\mu \in \mathcal{E}$

$$\langle a \,|\, b \rangle = a_\mu b^\mu = \eta_{\mu\nu} a^\mu b^\nu \tag{29}$$

and the Minkowski norm

$$||a^\mu|| = \sqrt{|a_\mu a^\mu|}, \tag{30}$$

where the absolute value under the square root is necessary because the Minkowski metric is not positive definite. It defines three classes of vectors that can be summarized in the light cone (see figure 3): there are

- space-like vectors: $\mathrm{d}s^2 > 0$,
- time-like vectors: $\mathrm{d}s^2 < 0$,
- and light-like vectors: $\mathrm{d}s^2 = 0$,

and from every point one can draw the cone in two directions, the future and the past cone, respectively.

With those ingredients we are able to define *Minkowski Space-time* M^4 as the 4-tuple consisting of

1. a 4 dimensional affine space $\mathcal{E}$ over $\mathbb{R}$ with underlying vector space E,
2. a metric tensor $g_{\mu\nu}$, as defined above,
3. a chosen forward direction, and
4. a chosen orientation.

Having defined the mathematical space that is suitable to describe physics from inertial frames, we can define the set of transformations that map any inertial frame Σ to another Σ'

$$A = \{\mathcal{M} : M^4 \to M^4, \Sigma \mapsto \Sigma' = \mathcal{M}(\Sigma) \,|\, \Sigma, \Sigma' \text{are inertial}\} \tag{31}$$

which is called *affine group*.

Let us investigate the elements of A or better its subgroups by their physical interpretation: The subgroup that carries the crucial elements that distinguishes the world of special relativity from that of Newtonian mechanics is the Lorentz group O(3,1).[33] Its elements are Lorentz transformations Λ which are defined as these $\mathcal{M} \in A$ that leave the inner product invariant

$$\langle a \,|\, b\rangle = \langle \Lambda(a) \,|\, \Lambda(b)\rangle \quad \forall\, a, b \in M^4. \tag{32}$$

The most important subgroup of O(3,1) is the restricted Lorentz group $\mathrm{SO}_o(3,1)$ that is the intersection of the *proper Lorentz group* SO(3,1) that preserves the chosen orientation of M^4 and the *orthochronous Lorentz group* $\mathrm{O}_o(3,1)$ that preserves the chosen time direction. It is *continuously connected* to the identity, which means that any element of $\mathrm{SO}_o(3,1)$ can be constructed by the repeated application of infinitesimal transformations. The connection between $\mathrm{SO}_o(3,1)$ and the full O(3,1) is given by the so-called discrete transformations, which consist of *reflections* in time (time reversal $\mathcal{T}$) and space (parity $\mathcal{P}$). A possible representation that acts on Minkowski 4-vectors $x^\mu \in M^4$ would be

$$\mathcal{T} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \mathcal{P} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{33}$$

From the given arguments, we know that we only need to study $\mathrm{SO}_o(3,1)$ in the following. $\mathrm{SO}_o(3,1)$ is a noncompact non-Abelian Lie group of dimension 6. Its generators are the three infinitesimal transformations L_1, L_2, L_3 of rotations $\mathcal{R}$ that by their own form the

[33] In contrast to the Galilean group in Newton theory.

subgroup SO(3) of $\mathrm{SO}_o(3,1)$. Its Lie-Algebra is

$$[L_i, L_j] = \mathbf{i}\epsilon^{ijk} L_k \quad i,j,k = 1,2,3. \tag{34}$$

The other generators are the three infinitesimal transformations K_1, K_2, K_3 of Lorentz boosts $\mathcal{K}$. They do not form a subgroup of $\mathrm{SO}_o(3,1)$, because their Lie-Algebra

$$[K_i, K_j] = -\mathbf{i}\epsilon^{ijk} L_k \quad i,j,k = 1,2,3 \tag{35}$$

shows that two boosts in different directions form a rotation. Finally the Lie-Algebra between both

$$[L_i, K_j] = \mathbf{i}\epsilon^{ijk} K_k \quad i,j,k = 1,2,3. \tag{36}$$

completes the Lie-Algebra of $\mathrm{SO}_o(3,1)$. We give as example their differential representation which acts on the space of differentiable functions over M^4

$$\vec{L} \equiv \begin{pmatrix} L_1 \\ L_2 \\ L_3 \end{pmatrix} = -\mathbf{i} \begin{pmatrix} x^1 \\ x^2 \\ x^3 \end{pmatrix} \times \begin{pmatrix} \partial_1 \\ \partial_2 \\ \partial_3 \end{pmatrix} = \mathbf{i}\vec{x} \times \nabla, \tag{37}$$

$$\vec{K} \equiv \begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix} = -\mathbf{i} \begin{pmatrix} x^0\partial_1 + x^1\partial_0 \\ x^0\partial_2 + x^2\partial_0 \\ x^0\partial_3 + x^3\partial_0 \end{pmatrix}. \tag{38}$$

As noted in the last subsection, a Lie-Algebra does not always map one-to-one to a Lie-group and this is also the case for $\mathrm{SO}_o(3,1)$. Its respective covering group is called SL(2), which can be defined as the group of rotations in the complex plane. The map between both is two-to-one and that is why $\mathrm{SO}_o(3,1)$ is called doubly-covered. This has important implications: The Casimir invariants that label the irreducible representations are those of the covering group SL(2). Hence, the double cover means that for $\mathrm{SO}_o(3,1)$ there are instead two labels necessary for every invariant. Later in this subsection, we introduce the Casimir invariants of SL(2) properly, but we want to anticipate that one of those is directly connected to the square of the angular-momentum operator, that is known from non-relativistic quantum mechanics. Its eigenvalues hence label the irreducible representations of SL(2) and so its possible spinor-realizations.[34] The eigenvalues are integer or half-integer valued which correspond to the intrinsic spin of the respective field. From non-relativistic quantum mechanics, we already know that the half-integer values are not realized for angular-momentum states. For example, the hydrogen atom exhibits only integer quantum numbers. The reason why the half-integer spinor representations are realized in Minkowski space is exactly that the Poincaré symmetries are doubly covered

[34] For details, see for example Lyubarskii [2013].

by SL(2). Thus, the two abstract labels can be interpreted as denoting the particle or antiparticle part of the spinor, respectively. Hence, also antiparticles are the consequence of the particular properties of relativistic space-time symmetry.

This induces another type of discrete symmetry transformation, which is the exchange of both labels or the exchange of particle and antiparticle. We call this *charge conjugation* $\mathcal{C}$. Its representation in the space of Minkowski 4-vectors is trivially the identity matrix, which means that a field that would be described by Minkowski 4-vectors does not have an antiparticle or is its own antiparticle. This is also the case for the 3-vectors belonging to photons with spin 1. A non-trivial representation of $\mathcal{C}$ can be found for Dirac spinors that we want to mention for completeness

$$\mathcal{C}\psi\mathcal{C}^{-1} = \gamma^0\psi^* = \bar{\psi}^T. \tag{39}$$

In Greiner et al. [2013, ch. 10.3.2], the implications of this definition are well illustrated and it is shown that it really interchanges particle and anti-particle. We finally want to emphasize that $\mathcal{C}$ is not part of SO(3,1) but it is obviously very connected to it. This is expressed in the famous *CPT-theorem*.[35] The CPT-theorem states under very loose assumptions that every quantum field theory that is Lorentz covariant must be invariant under the simultaneous application of $\mathcal{C}, \mathcal{P}$ and $\mathcal{T}$.

To complete the survey about the affine group A, there is only one last part left, which is the 4 dimensional Lie group of translations $\mathcal{T}$, that map a vector $x^\mu \in M^4$ to another $x'^\mu \in M^4$:

$$\mathcal{T}(x^\mu) = x'^\mu = x^\mu + a^\mu, \tag{40}$$

where a^μ is a constant interconnecting vector. It is Abelian and hence its generators P_μ have the trivial Lie-Algebra

$$[P_\mu, P_\nu] = 0 \quad \mu, \nu = 0, 1, 2, 3. \tag{41}$$

The respective differential representation is

$$P_\mu = \mathbf{i}\partial_\mu. \tag{42}$$

Both together finally form the *Poincaré group* IO(3,1) (or inhomogeneous Lorentz group), which is the *minimal subgroup* of A. To complete its Lie-Algebra, we need to add to

[35] The CPT-theorem was proved independently by different people, but for example by Bell [1954]

equations (34) to (36) and (42) the commutators between O(3,1) and $\mathcal{T}$

$$\begin{aligned}
[L_i, P_0] &= 0 \quad i = 1, 2, 3, \\
[L_i, P_j] &= \mathbf{i}\epsilon_{ijk} P_k \quad i, j = 1, 2, 3, \\
[K_i, P_0] &= -\mathbf{i} P_i \quad i = 1, 2, 3, \\
[J_i, P_j] &= \mathbf{i}\delta_{ij} P_0 \quad i, j = 1, 2, 3.
\end{aligned} \tag{43}$$

As already mentioned, ISO(3,1) has two Casimir invariants, the momentum square

$$P_\mu P^\mu \tag{44}$$

that is proportional to the *mass* of a field[36] and the square of the *Pauli-Lubanski pseudovector*

$$\begin{aligned}
& W_\mu W^\mu, \\
\text{with } & W_0 = J_i P_i, \\
& W_i = J_i - \epsilon_{ijk} P_j K_k
\end{aligned} \tag{45}$$

that can be associated to the spin of the respective field.[37] The already mentioned implications of the double cover of the Lorentz group are integrated in the spin label: for half-integer spins there are so called left-handed and right-handed labels possible.[38] It was *E. Wigner* who first discovered that this means that every quantum field of the standard model can be categorized by its mass and spin (*Wigner's classification*).

An electronic field spinor Ψ belongs to the irreducible representation of ISO(3,1) that has $p_\mu p^\mu = m_e c^2$ and $W_{mu} W^\mu = M_e^2 s_e(s_e + 1)$ with the electron mass $m_e = 9,109 \cdot 10^{-31}$ and the electron spin $s_e = 1/2$ for the left- and right-handed label. Its so defined transformation properties make it a Dirac spinor and it evolves due to the respective covariant field equation, which is the Dirac equation. A Maxwell field spinor Φ consequently belongs to the irreducible representation with $p_{mu} p^\mu = 0$ and $W_0 W^0 / p_i p^i = s_{ph}$ with the photon spin $s_{ph} = 1$. There is no difference between left- and right-handed label and Φ has the transformation properties of a normal 3-vector. Its evolution is given through Maxwell equations.[39]

Lastly, we shortly want to discuss the implications of Noether's theorem that are implicitly already integrated in the definitions of the generators of ISO(3,1). The theorem states

[36] It could be called the group theoretical embodiment of the relativistic mass-shell-constraint.

[37] For details see for example Niederer and O'Raifeartaigh [1974].

[38] Interestingly it turns out that for integer spins there is no difference between the right- and the left-handed label. For more detailed discussion see Schwichtenberg [2015].

[39] A detailed derivation of these admittedly very short statements, including the different forms of W_{mu} are given in Niederer and O'Raifeartaigh [1974].

that if any equation of motion is fully (and not form) invariant under certain symmetries, it exhibits conservation laws. A certain symmetry is always connected to the same conservation law and the respective pairs are shown in table 1. This is also the tool to interpret the group theoretical quantities: A translation by a_μ of a state $|\Phi\rangle$ for example is generated by the infinitesimal momentum operator through the exponential map

$$\mathcal{T}_a |\Phi\rangle = e^{-\mathbf{i}a_\mu P^\mu} |\Phi\rangle . \tag{46}$$

If $|\Phi\rangle$ is translationally invariant, then its momentum cannot change, so especially the Energy $E = P_0$ is conserved over time $t = a_0$.

Symmetry	Conservation of
Rotations $\mathcal{R}$	Angular Momentum
Boosts $\mathcal{K}$	Center of Energy
Translations $\mathcal{T}$ - spatial	Momentum
Translations $\mathcal{T}$ - temporal	Energy

TAB. 1: Conservation laws according to the different types of Poincaré transformations.

2.3.3 Gauge Invariance

In this last subsection about the symmetries of QED, we want to introduce gauge symmetry, the last type of symmetry group that is important for quantum electrodynamics. We eventually show how the QED Lagrangian with minimal coupling can be deduced from imposing local gauge invariance on the Dirac theory.

We saw that Poincaré invariance is sufficient to classify all fundamental fields and to find their equations of motion. For QED, we still need to find the right description of the interaction between the so derived free Dirac and Maxwell fields. This also can be done very elegantly by postulating a symmetry of a very different type, which is gauge symmetry. it is common knowledge that gauge symmetry is more a formal description of a mathematical redundancy instead of the property of a real physical object. But interestingly, it turns that every theory of the standard model exhibits certain gauge symmetry and their descriptions can be based on the assumption of local gauge invariance. Formally this is done by defining the fields on so-called *fibre-bundles* that can roughly be interpreted as the freedom of choosing arbitrary reference frames at every point. The typical derivation is done in the action description that is especially suited for symmetry considerations. To find the QED action we start with the Dirac part

$$S_D = \int \mathrm{d}^4x \bar{\psi} \left(\mathbf{i}\hbar c \gamma^\mu \partial_\mu - mc^2 \right) \psi, \tag{47}$$

and require local U(1) gauge invariance, which means that the action is invariant under

arbitrary local phase transformations of the field ψ[40]

$$\psi \to \psi' = \psi e^{\mathbf{i}\Theta(x^\mu)} \quad \Rightarrow \quad S' = S \tag{48}$$

The term that arises from the derivative term is then countered by introducing the appropriate *covariant derivative*

$$D_\mu = \partial_\mu - \mathbf{i}\frac{e}{\hbar}A_\mu \tag{49}$$

with a new gauge field A_μ. This introduces *minimal coupling*

$$\mathcal{L}_{int} = e\bar{\psi}\gamma^\mu\psi A_\mu. \tag{50}$$

In the most general case, we must treat A_μ as independent field and find its free Lagrangian. There are several possibilities to do so, but in the QED case, there are good arguments (e.g. dimensional reasons) that the free Lagrangian is found by means of the *Yang-Mills theory* [Yang and Mills, 1954]. The corresponding term is exactly the free Maxwell Lagrangian

$$\mathcal{L}_{MW} = -\frac{1}{4\mu_0}F^{\mu\nu}F_{\mu\nu}, \tag{51}$$

if e is identified with the electric charge of an electron and μ_0 with the permeability of free space.

As for every symmetry, there is a conservation law associated to gauge invariance. It is the (local) conservation of charge, which is embodied in the continuity equation

$$\partial_\mu j^\mu = 0 \tag{52}$$

for the electric current

$$j^\mu = e\bar{\psi}\gamma^\mu\psi. \tag{53}$$

In equation (52) contained, we find also the (global) conservation of charge

$$Q = \int \mathrm{d}^3x\, j^0 = const, \tag{54}$$

which refers to global gauge invariance. Already the free Dirac theory has this weaker form of gauge symmetry, so the charge of a free Dirac field is also conserved.

[40] It is also called *internal* symmetry, as it refers to transformations of the field itself and not of the coordinates.

3 Accessing QED by Means of Time Translations

As shown in the last chapter that there are a lot of different frameworks to study QED. Most important in perturbative approaches was for example the S-Matrix. Lattice gauge theory is typically formulated by means of the path integral formalism.[41] Therefore, this entire chapter is devoted to the framework that is the basis of the topic of this thesis: our space- and time-resolved model in real-space. The model is a Hamiltonian-based approach, so the first section 3.1 is about the construction of a QED-Hamiltonian. The second section (3.2) reviews the canonical quantization procedure in continuous momentum space, which is a well-developed formalism for the free Maxwell and Dirac theory. It serves as reference for our formalism that also makes use of the second quantization procedure, but in a different way. The idea to derive the discretized version of a quantum field theory by a mode expansion is sketched in the last section (3.3) of this chapter.

3.1 A QED Hamiltonian

In this section we want to present the main tool for our model: the Hamiltonian. We shortly explain the difficulties of distinguishing the time axis in a relativistically invariant theory (subsection 3.1.1). The second subsection 3.1.2 discusses the problems and aspects of the derivation of a QED Hamiltonian, especially within the usual framework of Lagrange theory. In the last subsection (3.1.3), we present a different approach, introduced by Bialynicki-Birula and Bialynicka-Birula [1984], that does not involve a Lagrangian at all and that was followed during the derivation of our model. Of course, the Hamiltonians are equivalent in both approaches.

3.1.1 What Means Hamiltonian in Minkowski Space?

As QED is a relativistically invariant theory one may question the need of a Hamiltonian that, being conjugate to time translations, violates the relativistic principles by distinguishing one coordinate. In fact, there are a lot of approaches that do not necessarily need a Hamiltonian. For calculations with propagator theory for example, one typically works directly with the Lagrangian. But looking at more or less all other research fields that are described on a (relativistic or non-relativistic) quantum mechanical level, one finds Hamiltonian based approaches. Consequently, the advantage of a QED Hamiltonian is that one can apply and compare results to a whole arsenal of techniques that where developed in the last century.

[41] It was not introduced, but the reader is referred to [Lin and Meyer, 2014].

3.1.2 Discussion of the Derivation

How can we derive such a relativistic Hamiltonian? The typical way in (non-relativistic theories) would be the Legendre transformation of the velocity variables of the Lagrangian. This is not trivially transferable to a relativistic theory. The reason is simply the fact that the four degrees of freedom of spacetime, that the relativistic action principle necessarily allows for, need to be constraint: also a relativistic field (or particle) can only move in three directions. This is encoded in the fundamental mass-shell constraint

$$p^\alpha p_\alpha = m^2 c^2 \tag{55}$$

of the four-momenta of a field (or particle) with restmass $m \geq 0$.[42] This can also be interpreted as a fundamental gauge invariance of relativistic theories. The gauge fixing corresponds to a certain coordinate choice, especially to the choice of the *time* parameter. To put it differently, although we can choose space and time coordinates arbitrarily, we have to choose them. But it is possible to treat such Legendre transformations under constraints. Dirac for example developed complicated techniques to integrate the constraints of relativistic space-time in the Hamiltonian formalism and based on this has formulated a canonical quantum field theory [Dirac, 1964].

3.1.3 A Different Approach

We discussed the problems of deriving a meaningful Hamiltonian within a Lagrangian theory. In this subsection, we want to follow a different approach formulated by Bialynicki-Birula and Bialynicka-Birula [1984]. Birula directly postulates the Hamiltonian together with the Heisenberg equations of motion. Hence, no Legendre transformations under constraints and even no Lagrangian at all are involved. Instead the Hamiltonian is "smartly guessed" first and then justified post-hoc by the derivation of the coupled Dirac and Maxwell equations, comparably to the Lagrangian theory. The derivation itself is done by means of the postulated Heisenberg equation. The equivalent in Lagrangian theory would be the least-action principle.

The starting point of the theory is the emphasis on energy being "undoubtedly, the most important and universal physical quantity" [Białynicki-Birula et al., 2013, sec. 2, p. 41]. This implies the emphasis on the time translations, which is embodied in the Heisenberg equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t} F = \frac{1}{\mathbf{i}\hbar}[F, H], \tag{56}$$

[42] For particles without restmass, like the photon, there is even one more constraint. This complicates the situation even more. We turn to that in subsection 3.2.2.

for any observable F.[43].

Then we take into account the free limits (coupled to external sources, equations (1) and (3)), that give us already the desired full equations, when we interpret the external as the respective internal fields.[44]

Before we can postulate a well-defined Hamiltonian, we must apply a gauge condition to the vector four-potential $A^\alpha = (A^0, \vec{A})$. This is due to the same reasons that already complicated the quantization of the Maxwell field. As photons have rest-mass zero, there is no canonical conjugate to the A^0 component of the four-potential. The canonical quantization is only possible within a certain gauge. $\vec{A}$ is invariant under U(1) gauge transformations

$$\vec{A} \to \vec{A}' = \vec{A} + \nabla \cdot \xi, \quad A^0 \to A'^0 = A^0 + \frac{\partial}{\partial t}\xi \tag{57}$$

with any differentiable gauge function ξ. The latter equation shows that in the new approach: without gauge condition, the time translations of A^0 would not be uniquely defined.[45]

To make time translations well-defined, we impose the minimal time-dependent gauge condition

$$A^0 = 0, \tag{58}$$

that fixes the time choice but still leaves all spatial gauge freedom. Hence it is referred to as temporal gauge.[46]

With the gauge condition, we can perform the canonical quantization. The canonical field pairs are the Dirac-spinor and its Hermitian conjugate $\hat{\psi}, \hat{\psi}^+$ and the spatial three-vector of the vector potential $\hat{\vec{A}}$ and its temporal derivative, the electrical field $\hat{\vec{E}}$. Now these are treated as operators in Hilbert space and we postulate their canonical (anti-)commutation relations[47]

$$\begin{aligned} \left[\hat{\psi}_\lambda(\vec{r}), \hat{\psi}^+_{\lambda'}(\vec{r}')\right]_+ &= \delta_{\lambda\lambda'}\delta(\vec{r} - \vec{r}'), \\ \left[\hat{A}_\mu(\vec{r}), \hat{E}_{\mu'}(\vec{r}')\right] &= \mathbf{i}\,\delta_{\mu,\mu'}\delta(\vec{r} - \vec{r}'). \end{aligned} \tag{59}$$

[43] This is of course not a mathematically sufficient definition. Later F and H will become operators in Hilbert space.

[44] This was discussed in subsection 2.1.1.

[45] This is a different ambiguity than the already mentioned one arising from the coordinate choice. Hence, there are always two reasons for not well-defined time propagation in a covariant gauge theory: Lorentz-covariance guarantees for no distinguished time axis in Minkowski space, Gauge invariance guarantees for no excellent "position" choice in the fiber bundle. The former one was actually already done implicitly because for definition of the fields and their derivatives we had to choose an inertial frame.

[46] The importances of the gauge condition in the quantization process is a long known issue. It is discussed on a general level for example here Strocchi [2004].

[47] The anti-commutator is marked by a +-sign.

All other commutators vanish. Finally, we postulate the canonical Hamiltonian[48]

$$\hat{H} = \int_{\mathbb{R}^3} \frac{1}{2} \left[\hat{\psi}^+, \left(mc^2 \underline{\beta} - \mathbf{i}\hbar c \, \underline{\vec{\alpha}} \cdot \nabla - e \, \underline{\vec{\alpha}} \cdot \vec{A} \right) \hat{\psi} \right] + \frac{\epsilon_0}{2} \left(\left(\nabla \times \hat{\vec{A}} \right)^2 + \left(c\hat{\vec{E}} \right)^2 \right) \mathrm{d}^3 r, \quad (60)$$

where the original Dirac notation was used

$$\underline{\beta} = \gamma^0 = \mathrm{diag}(1, 1, -1 - 1), \; \underline{\alpha_i} = \gamma^0 \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad (61)$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; \sigma_y = \begin{pmatrix} 0 & -\mathbf{i} \\ \mathbf{i} & 0 \end{pmatrix}, \; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (62)$$

We show the consistency of our postulates by deriving the correct field equations:

$$\begin{aligned}
\partial_t \hat{\psi} &= \frac{1}{\mathbf{i}\hbar}[\hat{\psi}, \hat{H}] = \frac{1}{\mathbf{i}\hbar} \left[m\underline{\beta} - \mathbf{i}\hbar c \, \underline{\vec{\alpha}} \cdot \nabla - e \, \underline{\vec{\alpha}} \cdot \hat{\vec{A}} \right] \hat{\psi}, \\
\partial_t \hat{\psi}^+ &= \frac{1}{\mathbf{i}\hbar}[\hat{\psi}^+, \hat{H}] = -\frac{1}{\mathbf{i}\hbar} \hat{\psi}^+ \left[m\underline{\beta} + \mathbf{i}\hbar c \, \underline{\vec{\alpha}} \cdot \overleftarrow{\nabla} - e \, \underline{\vec{\alpha}} \cdot \hat{\vec{A}} \right], \\
\partial_t \hat{\vec{A}} &= \frac{1}{\mathbf{i}\hbar}[\hat{\vec{A}}, \hat{H}] = -\hat{\vec{E}}, \\
\partial_t \hat{\vec{E}} &= \frac{1}{\mathbf{i}\hbar}[\hat{\vec{E}}, \hat{H}] = \nabla \times (\nabla \times \hat{\vec{A}}) - \hat{\vec{j}},
\end{aligned} \quad (63)$$

where $\overleftarrow{\nabla}$ indicates the derivative acting to the left and $\hat{\vec{j}}$ is the spatial part of the electric current density

$$\hat{j^\mu} = \frac{1}{2}[\hat{\bar{\psi}}, \gamma^\mu \hat{\psi}] = (\hat{j^0}, \hat{\vec{j}}). \quad (64)$$

Crucially, we did not use the full gauge freedom to derive (60), we just made sure that the time evolution is well-defined. It is still possible to choose pure spatial gauges to remove unphysical solutions that would violate the Gauss law.

3.2 Mode Expansions in Quantum Field Theory

Before introducing our approach, we briefly want to recapitulate the usual second quantization procedure for the Maxwell and the Dirac field. Throughout this section, Greiner et al. [2013] served as general source, when not indicated otherwise.

[48] In the quantized theory, the commutator in the Dirac part is necessary for charge conjugation invariance. Typically this is done through normal-ordering. See for example Zakir [2007]

3.2.1 Dirac-Field

We start with the Dirac field ψ[49] that obeys the transformation laws of a relativistic spinor. Its (classical) time evolution is determined by the free Dirac-Equation

$$(\mathbf{i}\hbar\gamma^\mu\partial_\mu - mc)\,\psi = 0. \tag{65}$$

It can be derived from an action principle with the Lagrange density

$$\mathcal{L}_{Dirac} = \bar{\psi}\left(\mathbf{i}\hbar c\gamma^\mu\partial_\mu - mc^2\right)\psi \tag{66}$$

where $\bar{\psi} = \psi^+\gamma^0$ is the Lorentz covariant adjoint spinor. The field momenta are

$$\pi_\psi = \frac{\partial\mathcal{L}_{Dirac}}{\partial\dot{\psi}} = \mathbf{i}\psi^+ \quad \text{and} \quad \pi_{\psi^+} = \frac{\partial\mathcal{L}_{Dirac}}{\partial\dot{\psi}^+} = 0. \tag{67}$$

Through the corresponding Legendre-transformation and integration we derive the Hamiltonian

$$H_{Dirac} = \int \mathrm{d}^3r\,\psi^+\left(-\mathbf{i}\hbar c\,\underline{\vec{\alpha}}\cdot\nabla + mc^2\beta\right)\psi. \tag{68}$$

We quantize by treating the fields as operators and by postulating the anti-commutation relations

$$\left[\hat{\psi}_\lambda(\vec{x}), \hat{\psi}^+_{\lambda'}(\vec{x}\,')\right]_+ = \delta_{\lambda\lambda'}\delta(\vec{x}-\vec{x}'), \tag{69}$$

$$\left[\hat{\psi}_\lambda(\vec{x}), \hat{\psi}_{\lambda'}(\vec{x}\,')\right]_+ = \left[\hat{\psi}^+_\lambda(\vec{x}), \hat{\psi}^+_{\lambda'}(\vec{x}\,')\right]_+ = 0. \tag{70}$$

The next step is the mode expansion that is performed in the eigenbasis of the Dirac equation which is the set of *plane-wave solutions*[50]

$$\psi^s_{\vec{p}}(\vec{x},t) = (2\pi)^{-3/2}\sqrt{\frac{m}{\omega_p}}\omega_s(\vec{p})e^{-\mathbf{i}\epsilon_s(\omega_p t - \vec{p}\cdot\vec{x})}, \tag{71}$$

where r represents the spinor index. Arbitrarily $s = 1, 2$ was chosen to denote the positive energy solutions with $E = +\omega_p = \sqrt{\vec{p}^2 + m^2}$ and $s = 3, 4$ those with $E = -\omega_p = -\sqrt{\vec{p}^2 + m^2}$. To capture this and to write general solutions the sign function $\epsilon_s = \pm 1$ was introduced. One can show that they are normalized in a distributional sense

$$\int \mathrm{d}^3r\,(\psi^{s'}_{\vec{p}'})^+\psi^s_{\vec{p}} = \delta_{rr'}\delta^3(\vec{p}-\vec{p}'), \tag{72}$$

[49] We omit the spinor arrow $\vec{\psi} = \psi$.

[50] In this subsection, we change units to natural units as this is the usual way to present second quantization in relativistic theories.

where the special orthogonality and completeness relations for the unit-spinors ω_r was used. As those obey a spinor algebra, their momentum representation is not as trivial as for a vector. Especially they become momentum dependent[51].

The plane-wave expanded field operators read

$$\begin{aligned}\hat{\psi}(\vec{x},t) &= \sum_{r=1}^{4}\int \mathrm{d}^3p\,\hat{a}_s(\vec{p})\psi^s_{\vec{p}}(\vec{x},t),\\ \hat{\psi}^+(\vec{x},t) &= \sum_{r=1}^{4}\int \mathrm{d}^3p\,\hat{a}^+_s(\vec{p})\psi^{s+}_{\vec{p}}(\vec{x},t),\end{aligned} \tag{73}$$

with the creation and annihilation operators $\hat{a}, \hat{a}^+$. Their anti-commutation relations can be derived from those of the field operators

$$\begin{aligned}\left[\hat{a}_s(\vec{p}),\hat{a}^+_{s'}(\vec{p}\,')\right]_+ &= \delta_{ss'}\delta(\vec{p}-\vec{p}\,'),\\ \left[\hat{a}_s(\vec{p}),\hat{a}_{s'}(\vec{p}\,')\right]_+ &= \left[\hat{a}^+_s(\vec{p}),\hat{a}^+_{s'}(\vec{p}\,')\right]_+ = 0.\end{aligned} \tag{74}$$

The second quantized Hamiltonian can now be derived by inserting the expansion into (68)

$$\hat{H}_{Dirac} = \int \mathrm{d}^3p\left(\sum_{s=1}^{2}\omega_p\hat{a}^+_s(\vec{p})\hat{a}_s(\vec{p}) - \sum_{s=3}^{4}\omega_p\hat{a}^+_s(\vec{p})\hat{a}_s(\vec{p})\right), \tag{75}$$

where positive and negative energies have been separated. This Hamiltonian exhibits a lot of the typical problems of relativistic quantum field theories. It is not positive definite and so its spectrum is infinite in positive and negative direction. This implies that a definition of a ground-state and even the vacuum is not possible. The most prominent and first solution was due to Dirac with his “electron sea” construction (see figure 4): One interprets the Dirac equation as an effective equation that only describes missing electrons (”holes”) in a sea of infinite degrees of freedom as negative energy solution.

To formalize this process, a box normalization (regularization) is introduced to gain Kronecker-anti-commutators. Then the so-called vacuum energy which is the sum over all negative entries in H

$$E_0 = -\sum_{s=3}^{4}\sum_{\vec{p}}\omega_p \tag{76}$$

[51] See Greiner et al. [2013, p. 124] for details.

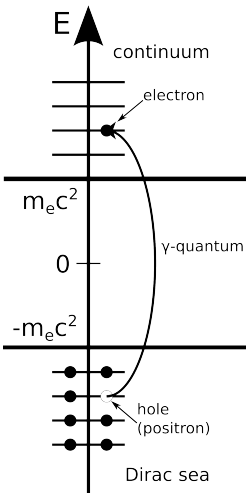

FIG. 4: The electron-positron picture due to Dirac is visualized: We assume a band of electron states with negative energy that is completely filled (Dirac sea). The measurable continuum is separated by a band gap of $\Delta E = 2m_e c^2$. An electron with positive energy in that continuum is created by the excitation of an electron in the negative band. The remaining hole behaves like an electron with reversed charge but positive energy. So it is called positron, the antiparticle of the electron.

is finite and can be subtracted from H

$$H' = H - E_0 = \sum_{\vec{p}} \left(\sum_{r=1}^{2} \omega_p \hat{a}_r^+(\vec{p}) \hat{a}_r(\vec{p}) - \sum_{r=3}^{4} \omega_p (1 - \hat{a}_r^+(\vec{p}) \hat{a}_r(\vec{p})) \right)$$
$$= \sum_{\vec{p}} \left(\sum_{r=1}^{2} \omega_p \hat{a}_r^+(\vec{p}) \hat{a}_r(\vec{p}) - \sum_{r=3}^{4} \omega_p \hat{a}_r(\vec{p}) \hat{a}_r^+(\vec{p}) \right). \tag{77}$$

This modified Hamiltonian H' is well-defined and positive-definite and also the vacuum state $|0\rangle$ can be defined as

$$n_{\vec{p},r} \, |0\rangle \, |_{r=1,2} = \bar{n}_{\vec{p},r} \, |0\rangle \, |_{r=3,4} = 0, \tag{78}$$

with the electron/positron number operators

$$n_{\vec{p},r} = \hat{a}_r^+(\vec{p}) \hat{a}_r(\vec{p}), \quad \bar{n}_{\vec{p},r} = \hat{a}_r(\vec{p}) \hat{a}_r^+(\vec{p}). \tag{79}$$

From these definitions one can see that $\hat{a}$ acts as annihilation operator for $r = 1, 2$ *but* as creation operator for $r = 3, 4$, which is a typical feature of charged theories. Therefore one usually labels the unit spinors by spin

$$\omega_1(\vec{p}) \equiv u(p, s), \quad \omega_2(\vec{p}) \equiv u(p, -s), \tag{80}$$
$$\omega_3(\vec{p}) \equiv v(p, -s), \quad \omega_4(\vec{p}) \equiv v(p, s), \tag{81}$$

and introduces new creation and annihilation operators for particles and antiparticles, respectively

$$\hat{a}_1(\vec{p}) \equiv \hat{b}(\vec{p}, s), \quad \hat{a}_2(\vec{p}) \equiv \hat{b}(\vec{p}, -s), \tag{82}$$

$$\hat{a}_3(\vec{p}) \equiv \hat{c}^+(\vec{p}, -s), \quad \hat{a}_4(\vec{p}) \equiv \hat{c}^+(\vec{p}, s). \tag{83}$$

Notably, the operators for the negative branch are defined as the hermitian conjugate. The expansion (73) reads (after performing the limit to infinite box size)

$$\hat{\psi}(\vec{x}, t) = \sum_s \int \frac{\mathrm{d}^3 p}{(2\pi)^{3/2}} \sqrt{\frac{m}{\omega_p}} \left(\hat{b}(\vec{p}, s) u(\vec{p}, s) e^{-\mathrm{i}\vec{p}\cdot\vec{x}} + \hat{c}^+(\vec{p}, s) v(\vec{p}, s) e^{+\mathrm{i}\vec{p}\cdot\vec{x}} \right), \tag{84}$$

and the new modified Hamiltonian is

$$H' = H - E_0 = \sum_s \int \mathrm{d}^3 p \, \omega_p \left(\hat{b}^+(\vec{p}, s) \hat{b}(\vec{p}, s) + \hat{c}^+(\vec{p}, s) \hat{c}(\vec{p}, s) \right), \tag{85}$$

which is probably the most common form of the Dirac Hamiltonian. One naturally can derive other operators from this expansion, for example the charge operator (54) that is important later

$$Q = e \int \mathrm{d}^3 x \, \hat{\psi}^+ \hat{\psi} \tag{86}$$

$$= e \sum_s \int \mathrm{d}^3 p \, \left(\hat{b}^+(\vec{p}, s) \hat{b}(\vec{p}, s) + \hat{c}(\vec{p}, s) \hat{c}^+(\vec{p}, s) \right). \tag{87}$$

By subtracting the vacuum charge Q_0, one can obtain an expression of the charge operator

$$\begin{aligned} Q' = Q - Q_0 &= e \sum_s \int \mathrm{d}^3 p \, \left(\hat{b}^+(\vec{p}, s) \hat{b}(\vec{p}, s) - \hat{c}^+(\vec{p}, s) \hat{c}(\vec{p}, s) \right) \\ &= e \sum_s \int \mathrm{d}^3 p \, \left(\hat{n}(\vec{p}, s) - \hat{\bar{n}}(\vec{p}, s) \right) \end{aligned} \tag{88}$$

that counts electrons positive and positrons negative as we want and thus can be seen as the post-hoc justification of our definitions. The momentum operator reads

$$\hat{\vec{P}} = \sum_s \int \mathrm{d}^3 p \, \vec{p} \left(\hat{n}(\vec{p}, s) + \hat{\bar{n}}(\vec{p}, s) \right), \tag{89}$$

so we confirm that the plane-wave expansion (73) is also eigenbasis of $\hat{\vec{P}}$. Interestingly, $\hat{\vec{P}}$ does not exhibit problems with negative energies as all contributions from commutations are canceled by the multiplication with $\vec{p}$ ($\int \mathrm{d}^3 p (\vec{p} \cdot 1) = 0$). Lastly, we want to mention the spin operator. It has a simple expression for so-called helicity states. They are

eigenfunctions of the helicity operator, that is defined as the projection of the angular momentum onto the direction of the momentum $\vec{p}$. This spin operator consequently is $\vec{p}$-dependent

$$\hat{S}_{\vec{p}} = \frac{1}{2}\left(\hat{n}(\vec{p},+) - \hat{n}(\vec{p},-) + \hat{\bar{n}}(\vec{p},s) - \hat{\bar{n}}(\vec{p},s)\right). \tag{90}$$

This justifies post hoc the spin definitions made before.

Eventually, we want to mention that the process of subtracting the vacuum energy can be expressed equivalently by so-called *normal ordering*.[52] This means that all operators that contain positive frequencies (so for the just defined expansion (82) only annihilation operators) are shifted to the right. The normal-ordered form $:\hat{O}:$ of the operator $\hat{O} = aa^+$ then takes the form

$$:\hat{O}: = a^+a \tag{91}$$

3.2.2 Maxwell-Field

The canonical quantization procedure of the Maxwell-field is on the one hand easier than in the Dirac case, as one does not have to struggle with the antiparticle problem. On the other hand, we encounter new difficulties due to the zero rest-mass of the photon. We see this when we try to quantize the theory. The canonical field pair is the vector potential and its canonical momentum, which is the electric field for the spatial part but turns out to be zero for the time-component of the vector-potential. This must be prevented by imposing a gauge condition.

In the following, we see that the gauge choice is very important for the canonical quantization and up to today it is under discussion what this means for the properties of the quantum theory at all.[53]

We start the derivation by recapitulating Maxwell's equations for the free electromagnetic field tensor $F^{\mu\nu}$

$$\partial_\mu F^{\mu\nu} = 0 \tag{92}$$

$$\partial_\mu \epsilon^{\mu\nu\rho\sigma} F_{\rho\sigma} = 0. \tag{93}$$

The latter is automatically guaranteed by expressing $F^{\mu\nu}$ through the vector potential $F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$. From this definition one can directly deduce the gauge invariance of $A^\mu = (A^0, \vec{A})$: for any differentiable function Λ,

$$A'^\mu = A^\mu + \partial^\mu \Lambda \tag{94}$$

[52] Or with the aid of a commutator, see footnote 48.
[53] See for example Strocchi [2004].

leads to the same field tensor as A^μ. To proceed, we need a Lagrangian that corresponds to (92), which is the simplest Lorentz scalar that we can construct from the field tensor

$$\begin{aligned}\mathcal{L}_{MW} &= -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} \\ &= \frac{1}{2}((-\partial_t\vec{A} - \nabla\cdot\vec{A})^2 - (\nabla\times\vec{A})^2) = \frac{1}{2}((\vec{E})^2 - (\vec{B}^2).\end{aligned} \tag{95}$$

When we want to construct a Hamiltonian through the Legendre transformation, we encounter the already mentioned problems: The vector potential carries 4 degrees of freedom whereas the actual photon field has only 2 polarizations. One reason is the artificial inclusion of time as a free parameter, and the second one is that photons do not have a free "mass parameter." Usually the theory is quantized in Lorentz gauge or Coulomb gauge. In the first case, one cannot impose the gauge before the quantization, because this would lead to wrong commutation relations. As a consequence, one needs to impose the gauge after the quantization as an operator condition on the state vectors

$$\langle\Phi|\partial_\mu A^\mu = 0|\Phi\rangle = 0. \tag{96}$$

Put differently, we span the whole Hilbert space and allow all kinds of unphysical solutions and afterwards just look at the physical states. This method was first introduced by Gupta [1950] and Bleuler [1950] and is a tool that is often consulted to apply constraints on a quantum theory.

Here we want to present a simpler but not covariant way of quantization. We impose the so-called radiation gauge

$$\nabla\cdot\vec{A} = 0, \quad A^0 = 0, \tag{97}$$

which corresponds to Coulomb and temporal gauge together in a certain inertial frame. Then the canonical conjugate to $\vec{A}$ is well-defined because the 0-component of A^μ was set to zero. We find

$$\pi_{\vec{A}} = \frac{\partial\mathcal{L}_{MW}}{\partial_t\vec{A}} = \partial_t\vec{A} = \vec{E}. \tag{98}$$

This expression makes clear that the imposed transversality from $\vec{A}$ transfers to its canonical momentum $\vec{E}$. Consequently, there are only 3 independent variables and finally we can construct a Hamiltonian

$$H_{MW} = \int \mathrm{d}^3x \frac{1}{2}\left((\partial_t\vec{A})^2 + (\nabla\times\vec{A})^2\right) = \int \mathrm{d}^3x \frac{1}{2}\left(\vec{E}^2 + \vec{B}^2\right). \tag{99}$$

After having solved the first problem, we move to the next one, namely the proper definition of commutation relations. We quantize the theory in the usual way by treating the

canonical fields as operators but then we have to postulate transverse delta[54] commutators

$$\left[\hat{E}^i(\vec{r}), \hat{A}^j(\vec{r}')\right] = -\mathbf{i}\,\delta_{\perp ij}(\vec{r}-\vec{r}') \tag{100}$$

as the 6 components of $\vec{A}$ and $\vec{E}$ are not independent. Here we can clearly see the non-local nature of photons in real space. The expressions become much easier in momentum space and this is an important reason why QED is normally treated in k-space. For that we introduce the plane-wave expansion

$$\begin{aligned}
\hat{\vec{A}}(\vec{x},t) &= \int \frac{\mathrm{d}^3k}{\sqrt{2\omega_k(2\pi)^3}} \sum_{\lambda=1}^{2} \vec{\epsilon}_\lambda(\vec{k}) \left(\hat{a}_{\lambda\vec{k}} e^{-\mathbf{i}\vec{k}\cdot\vec{x}} + \hat{a}^+_{\lambda\vec{k}} e^{\mathbf{i}\vec{k}\cdot\vec{x}}\right), \\
\hat{\vec{E}}(\vec{x},t) &= \int \frac{\mathrm{d}^3k}{\sqrt{2\omega_k(2\pi)^3}} \sum_{\lambda=1}^{2} \mathbf{i}\omega_k \vec{\epsilon}_\lambda(\vec{k}) \left(\hat{a}_{\lambda\vec{k}} e^{-\mathbf{i}\vec{k}\cdot\vec{x}} - \hat{a}^+_{\lambda\vec{k}} e^{\mathbf{i}\vec{k}\cdot\vec{x}}\right),
\end{aligned} \tag{101}$$

which looks different than for the Dirac ansatz (73) because the fields are real valued.[55] We interpret the prefactors as creation and annihilation operators and find

$$\begin{aligned}
[\hat{a}_{\lambda\vec{k}}, \hat{a}^+_{\lambda'\vec{k}'}] &= \delta_{\lambda\lambda'}\delta^3(\vec{k}-\vec{k}'), \\
[\hat{a}_{\lambda\vec{k}}, \hat{a}_{\lambda'\vec{k}'}] &= [\hat{a}^+_{\lambda\vec{k}}, \hat{a}^+_{\lambda'\vec{k}'}] = 0
\end{aligned} \tag{102}$$

for the respective commutation relations and

$$\hat{H}_{MW} = \int \mathrm{d}^3x\, \frac{1}{2} :\hat{\vec{E}}^2 + (\nabla\times\hat{\vec{A}})^2: \tag{103}$$

$$= \int \mathrm{d}^3k\, \omega_k \sum_{\lambda=1}^{2} \hat{a}^+_{\lambda\vec{k}} \hat{a}_{\lambda\vec{k}} \tag{104}$$

for the normal-ordered Hamiltonian where the vacuum energy was removed. The momentum operator is

$$\hat{\vec{P}} = \int \mathrm{d}^3x :\hat{\vec{E}}\times(\nabla\times\hat{\vec{A}}): = \int \mathrm{d}^3k \sum_{\lambda=1}^{2} \vec{k}\, \hat{a}^+_{\lambda\vec{k}} \hat{a}_{\lambda\vec{k}} \tag{105}$$

and finally one can define a spin operator

$$\hat{S}^{nl} = \mathbf{i} \int \mathrm{d}^3k \sum_{\lambda,\lambda'=1}^{2} \epsilon^n_{\lambda'}(\vec{k})\epsilon^l_\lambda(\vec{k}) \left(\hat{a}^+_{\lambda\vec{k}}\hat{a}_{\lambda'\vec{k}} - \hat{a}^+_{\lambda'\vec{k}}\hat{a}_{\lambda\vec{k}}\right) \tag{106}$$

[54] It is defined as the transverse projection of the 3D delta distribution $\delta_{\perp ij}(\vec{r}-\vec{r}') = (\delta_{ij} - \partial_i \frac{1}{\Delta}\partial_j)\delta^3(\vec{r}-\vec{r}')$. It has a Fourier representation $\delta_{\perp ij}(\vec{r}-\vec{r}') = \int \frac{\mathrm{d}^3k}{(2\pi)^3} e^{\mathbf{i}\vec{k}\cdot(\vec{x}-\vec{x}')}(\delta_{ij} - \frac{k_i k_j}{\vec{k}^2})$.

[55] Note that $\vec{E}$ is real despite the $\mathbf{i}$. This is actually the reason why there is the factor $-\mathbf{i}$ in the commutation relations, which is a general feature of uncharged (real) fields.

which can also be diagonalized by introducing helicity states with circular polarization modes.[56]

3.2.3 Coupled Maxwell-Dirac Case

We presented the eigen-representation of the Dirac and the Maxwell theory with all necessary complications. Generally speaking one can say that the free theories are more or less well understood, because we know these eigen-representations. The problems and also the interesting physics come with the interaction, which makes the theory non-linear and non-solvable. This can be well visualized by applying the eigen-representations on the coupling term. Hence, there is not much to say here but for completeness we want to show the representation of the coupling term

$$\begin{aligned}\hat{H}_{int} &= \hat{\psi}^{+}\hat{\psi}(\hat{\vec{\alpha}}\cdot\hat{\vec{A}}) \\ &= e\int \mathrm{d}^3x \sum_{r=1}^{4}\int \mathrm{d}^3p\, \hat{a}_s(\vec{p})\psi^s_{\vec{p}}(\vec{x},t)\sum_{r=1}^{4}\int \mathrm{d}^3p\, \hat{a}^{+}_s(\vec{p})\psi^{s+}_{\vec{p}}(\vec{x},t) \\ &\quad \hat{\vec{\alpha}}_{circular}\cdot\int \frac{\mathrm{d}^3k}{\sqrt{2\omega_k(2\pi)^3}}\sum_{\lambda=1}^{2}\vec{\epsilon}_\lambda(\vec{k})\left(\hat{a}_{\lambda\vec{k}}e^{-\mathbf{i}\vec{k}\cdot\vec{x}}+\hat{a}^{+}_{\lambda\vec{k}}e^{\mathbf{i}\vec{k}\cdot\vec{x}}\right), \end{aligned} \tag{107}$$

where $\hat{\vec{\alpha}}_{circular}$ is the representaiton of the α-Matrix in the respective circular frame that was also used for the mode expansion in $\vec{A}$.

We see, that the interaction terms becomes very complicated and especially non-local in the eigen-representation of the free fields. Every mode of the Dirac-field couples to every mode of the Maxwell field. This is another reason why we should formulate our theory in real-space.

3.3 Discretization as a Mode Expansion

After sketching the continuous Hamiltonian and the canonical quantization procedure, we now want to introduce the framework of our discretized theory. We perform this in a maybe unusual but very effective way. It allows for the discretization of any given Hamiltonian or operator and at the same time taking advantage of the language of canonical quantization.

Hence, we interpret the physical fields $|\Phi\rangle$ as operators

$$|\Phi\rangle \to \hat{\Phi}, \tag{108}$$

[56] See Greiner et al. [2013, p.165ff] for more details.

that act on number state vectors in Fock space $\mathcal{F}$

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} \mathcal{H}_n, \tag{109}$$

where $\mathcal{H}_n$ denotes an n-particle Hilbert space.

In the typical procedure in continuous quantum field theory, one expands these operators in any complete basis set like the eigenfunctions of the free theories

$$\hat{\Phi} = \sum_{i=0}^{\infty} \hat{a}_i \left|\phi_i\right\rangle, \quad \langle\phi_i|\phi_j\rangle = \delta_{ij}, \tag{110}$$

and interprets the coefficients as creation and annihilation operators, as shown in the last section (3.2). The discretization changes this crucially: we are not able to choose a complete basis because that would need arbitrary spatial resolution. Instead we have to truncate the basis to N functions

$$\hat{\Phi} = \sum_{i=0}^{N} \hat{a}_i \left|\phi_i\right\rangle. \tag{111}$$

This bandwidth-limited basis set is in contrast to the continuous case also well defined in real space.[57] We exploit this, to construct the theory on a more intuitive real-space grid. Here one should remark that this is an especially unfamiliar picture of photons that are not localizable.[58] However, in our approach it is possible to construct a "localized" photon on one grid site because of the bandwidth limitation.[59]

[57] Mode functions of the continuous real space are only defined in a distributional sense (delta distributions), which is not convenient as the multiplication of distributions is not well-defined. See [Schwartz, 1966].

[58] This can be shown very elegantly from a group theoretical point of view, see Rosewarne and Sarkar [1992].

[59] This is clear from the proof of Rosewarne and Sarkar [1992]: Localization means arbitrary precise position. A photon in any position interval hence is not localized.

4 Derivation of the Model

In this chapter, we finally want to introduce our model. We construct a discrete Hamiltonian-based theory, from which we are able to numerically investigate the complete, finite-dimensional Fock space of the theory.

We adopt the formalism of Birula, that was presented in subsection 3.1.3. It was shown there, that the QED Hamiltonian

$$\hat{H} = \int_{\mathbb{R}^3} \frac{1}{2} \left[\hat{\psi}^+, \left(mc^2 \underline{\beta} - \mathbf{i}\hbar c \, \underline{\vec{\alpha}} \cdot \nabla - e \, \underline{\vec{\alpha}} \cdot \vec{A} \right) \hat{\psi} \right] + \frac{\epsilon_0}{2} \left(\left(\nabla \times \hat{\vec{A}} \right)^2 + \left(c\hat{\vec{E}} \right)^2 \right) \mathrm{d}^3 r, \quad (60)$$

together with the Heisenberg equation of motion (56) leads to the right coupled field equations (63).

We see that the Hamiltonian is built by three ingredients: first, the Dirac spinors $\vec{\Psi}$, $\vec{\Psi}^+$ and the three-spinors (vectors) of the Maxwell field $\vec{A}, \vec{E}$, second, differential operators that act on the spinor, and third, some natural constants, which we directly adopt as being fundamental.

Let us first turn to the spinors. A "typical" discretization procedure would consist of discretizing the fields in any basis and approximating the differential operators by a finite-differences method. From the symmetry point of view (dicussed in section 2.3), one could think of going even one step back. We could try to discretize the Minkowski fibre-bundle and then construct spinors as finite irreducible representations from the discrete forms of Poincare and gauge symmetry. Unfortunately this is not possible, because there is no discrete grid that is in its continuum limit Poincare and gauge invariant simultaneously [Wilson, 1974].

Instead, we could break gauge symmetry and try to construct "discrete spinors" only from Poincaré transformations . But also this is not possible. There are discretized versions of the Poincaré group, that indeed have the correct continuous limit. But the transition between discrete and continuous theory is by itself not continuous. Only translations can be properly approximated to any order by a lattice. The subgroup of pure local Lorentz transformations instead, cannot properly be mapped to any space-time grid. But the spinor representation of the Poincaré group is mainly defined by the Lorentz group. Hence, there is not such a thing like a "discrete spinor." Consequently, the "typical" discretization procedure is in terms of the fields also the only possible. We have to distinguish between the two roles of Minkowski space: It defines the transformation properties of the spinors as a continuous space. But as the definition space of the spinor fields we use the discretized Minkowksi space. The discretization is formally done by a mode expansion. We present this in 4.1.

The other ingredient of the discretization procedure is the treatment of the differential

operators. On the discretized space-time of the spinor fields we can define a vector space of bounded functions with a proper inner product, that would be a finite Hilbert space. Hence, the standard method, finite-differences, is easily applicable. This is the content of section 4.2.

At this point, we want to mention that there is also an alternative way. From a group theoretical point of view, the differential operators are representations of the Poincaré group acting on a Hilbert space. We show in chapter 6 that there is a discrete analogue and derive the respective operators. We can even formulate a Hamiltonian theory with continuous transition to the continuum, because is its constructed by means of momentum generators. There is no representation of the Lorentz group with its bad limit behavior involved.

In the last section (4.3), we explain how to implement the model in a code and perform numerical studies. The results of these studies for finite-differences are the content of chapter 5.

4.1 Mode Expansion in Rectangle Functions

In this section we present the derivation of our discretized Hamiltonian in terms of the fields. We want to introduce our approach by using the advantages and tools of second (canonical) quantization for the discretization problem.

We first define the approximation of the 3D real-space. Let us consider a 3D box M of lengths L_x, L_y, L_z. It is divided into small boxes of the lengths $\Delta_x, \Delta_y, \Delta_z$ so that

$$L_x = \Delta_x N_x, \quad L_y = \Delta_y N_y, \quad L_z = \Delta_z N_z, \tag{112}$$

where N_x, N_y, N_z are the numbers of grid points in the three directions, respectively.

We introduce the following mode expansion of the field operators $\hat{\psi}, \hat{\psi}^+$ and $\hat{\vec{A}}, \hat{\vec{E}}$[60]

$$\hat{\psi}(\vec{r}) = \sum_{\vec{r}_n}^{\vec{N}} \sum_{\lambda=1}^{4} \vec{e}_\lambda \, \Theta^3_{\vec{r}_n}(\vec{r}) \, \hat{c}_{\lambda,\vec{r}_n}, \tag{113}$$

$$\hat{\psi}^+(\vec{r}) = \sum_{\vec{r}_n}^{\vec{N}} \sum_{\lambda=1}^{4} \vec{e}_\lambda \, \Theta^3_{\vec{r}_n}(\vec{r}) \, \hat{c}^+_{\lambda,\vec{r}_n}, \tag{114}$$

$$\hat{\vec{A}}(\vec{r}) = \sum_{\vec{r}_n}^{\vec{N}} \sum_{\mu=1}^{3} \vec{e}_\mu \left(\hat{a}_{\mu,\vec{r}_n} + \hat{a}^+_{\mu,\vec{r}_n} \right) \Theta^3_{\vec{r}_n}(\vec{r}), \tag{115}$$

[60] The derivation is made in the Schrödinger picture, so that all time information is shifted to the state vector.

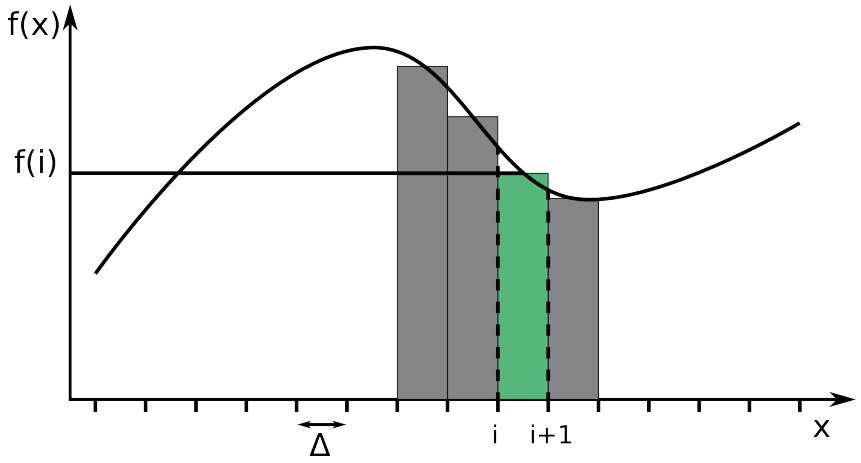

FIG. 5: The expansion in rectangle functions is illustrated: Any smooth function is approximated by piecewise constant steps.

$$\hat{\vec{E}}(\vec{r}) = \mathbf{i} \sum_{\vec{r}_n}^{\vec{N}} \sum_{\mu=1}^{3} \vec{e}_\mu \left(\hat{a}_{\mu,\vec{r}_n} - \hat{a}^+_{\mu,\vec{r}_n} \right) \Theta^3_{\vec{r}_n}(\vec{r}), \tag{116}$$

with the definitions:

$$\begin{aligned}
&\vec{N} = (N_x, N_y, N_z) && \rightarrow \text{ vector, referring to the number of sites,} \\
&\vec{r}_n = (x_n, y_n, z_n) && \rightarrow \text{ site counter for all 3 spatial dimensions,} \\
&\vec{e}_\lambda, \quad \vec{e}_\lambda \, \vec{e}_{\lambda'} = \delta_{\lambda\lambda'} && \rightarrow \text{ unit spinor for the 4 spinor entries,} \\
&\vec{e}_\mu, \quad \vec{e}_\mu \, \vec{e}_{\mu'} = \delta_{\mu\mu'} && \rightarrow \text{ unit vector for the 3 spatial components.}
\end{aligned}$$

The actual discretization is done by the mode functions, which are chosen as rectangle functions[61]

$$\begin{aligned}
&\Theta^3_{\vec{r}_n}(\vec{r}) = \Theta_{x_n}(x) \, \Theta_{y_n}(y) \, \Theta_{z_n}(z) \\
&\Theta_{r_{i,n}}(r_i) = \frac{1}{\sqrt{\Delta_{r_i}}} \Theta \left(\frac{\Delta_{r_i}}{2} - |r_i - r_{i,n}| \right) \\
&\int_M \Theta^3_{\vec{r}_n}(\vec{r}) \, \Theta^3_{\vec{r}_n{}'}(\vec{r}) \mathrm{d}^3 r = \delta_{\vec{r}_n \vec{r}_n{}'},
\end{aligned}$$

with $\{r_i\} = \{x, y, z\}$. In other words, this procedure samples continuous functions by a piecewise constant function as depicted in figure 5.

This discretization introduces a spatial bandwidth limitation. The minimal and maximal wavenumber k_i^{min}, k_i^{max} that can be resolved along each Cartesian direction ($i = x, y, z$)

[61] Also known as rectangular functions, see Wang, Ruye (2012). Introduction to Orthogonal Transforms: With Applications in Data Processing and Analysis. Cambridge University Press. p. 135-136

are

$$k_i^{min} = \frac{2\pi}{N_i}, \tag{117}$$

$$k_i^{max} = \frac{2\pi}{\Delta_{r_i}}. \tag{118}$$

In the limit of an infinitely large box $L_i \to \infty$ and infinitesimally small steps $\Delta_{r_i} \to 0$, we formally recover the continuous theory:[62]

$$\lim_{L_i\to\infty} \lim_{\Delta_{r_i}\to 0} \sum_{\vec{r}_n} \Theta^3_{\vec{r}_n}(\vec{r})\, \Theta^3_{\vec{r}_n}(\vec{r}\,') = \delta(\vec{r} - \vec{r}\,'). \tag{119}$$

4.1.1 Commutation Relations

To perform the canonical quantization, we need to derive new *discrete commutation relations* from the postulated ones (59). To find them, we project the field operator on one mode

$$\begin{aligned}\int \mathrm{d}^3 r \left(\vec{e}_\lambda \Theta^3_{\vec{r}_n}(\vec{r})\right) \hat{\psi}_{\lambda'}(\vec{r}) &= \sum_{\vec{r}_n}^{\vec{N}} \sum_{\lambda=1}^{4} \underbrace{\vec{e}_\lambda \vec{e}_{\lambda'}}_{\delta_{\lambda,\lambda'}} \underbrace{\int \mathrm{d}^3 r \Theta^3_{\vec{r}_n}(\vec{r})\, \Theta^3_{\vec{r}'_n}(\vec{r}\,')}_{\delta_{\vec{r}_n \vec{r}'_n}}\ \hat{c}_{\lambda',\vec{r}'_n} \\ &= \hat{c}_{\lambda,\vec{r}_n}.\end{aligned}$$

This gives us an expression for the annihilation operator

$$\hat{c}_{\lambda,\vec{r}_n} = \int \mathrm{d}^3 r \vec{e}_\lambda \Theta^3_{\vec{r}_n}(\vec{r}) \hat{\psi}_{\lambda'}(\vec{r}).$$

Similarly, for the creation operator one finds

$$\hat{c}^+_{\lambda,\vec{r}_n} = \int \mathrm{d}^3 r \vec{e}_\lambda \Theta^3_{\vec{r}_n}(\vec{r}) \hat{\psi}^+_{\lambda'}(\vec{r}).$$

Conveniently, we derive the same commutation relations like in the continuous theory

$$\begin{aligned}\left[\hat{c}_{\lambda,\vec{r}_n}, \hat{c}^+_{\lambda',\vec{r}_n\,'}\right]_+ &= \int \mathrm{d}^3 r \int \mathrm{d}^3 r' \vec{e}_\lambda \vec{e}_{\lambda'} \Theta^3_{\vec{r}_n}(\vec{r}) \Theta^3_{\vec{r}'_n}(\vec{r}\,') \underbrace{\left[\hat{\psi}_\lambda(\vec{r}), \hat{\psi}^+_{\lambda'}(\vec{r}\,')\right]_+}_{\delta_{\lambda\lambda'}\delta(\vec{r}-\vec{r}\,')} \\ &= \underbrace{\vec{e}_\lambda \vec{e}_{\lambda'} \delta_{\lambda\lambda'}}_{\delta_{\lambda\lambda'}} \int \mathrm{d}^3 r \Theta^3_{\vec{r}_n}(\vec{r}) \Theta^3_{\vec{r}'_n}(\vec{r}) \\ &= \delta_{\lambda\lambda'} \delta_{\vec{r}_n \vec{r}'_n}.\end{aligned}$$

[62] although there is not a well-defined real-space mode expansion as mentioned before.

All other anti-commutators vanish and altogether we have

$$[\hat{c}_{\lambda,\vec{r}_n}, \hat{c}_{\lambda',\vec{r}_n\,'}]_+ = \left[\hat{c}^+_{\lambda,\vec{r}_n}, \hat{c}^+_{\lambda',\vec{r}_n\,'}\right]_+ = 0, \tag{120}$$

$$\left[\hat{c}_{\lambda,\vec{r}_n}, \hat{c}^+_{\lambda',\vec{r}_n\,'}\right]_+ = \delta_{\lambda\lambda'}\delta_{\vec{r}_n\vec{r}'_n}. \tag{121}$$

The same (but slightly more complicated) method is applicable to the electromagnetic field,[63] but we can also just insert the mode expansion into the given commutation relations (59)

$$\begin{aligned}\left[\hat{E}_\mu(\vec{r}), \hat{A}_{\mu'}(\vec{r}\,')\right] &= \sum_{\vec{r}_n,\vec{r}'_n} \mathbf{i}\,\vec{e}_\mu\vec{e}_{\mu'}\Theta^3_{\vec{r}_n}(\vec{r})\,\Theta^3_{\vec{r}_n\,'}(\vec{r}\,') \underbrace{\left[\left(\hat{a}_{\mu,\vec{r}_n} - \hat{a}^+_{\mu,\vec{r}_n}\right), \left(\hat{a}_{\mu',\vec{r}_n\,'} + \hat{a}^+_{\mu',\vec{r}_n\,'}\right)\right]}_{\mathcal{C}} \\ &= \sum_{\vec{r}_n,\vec{r}'_n} \mathbf{i}\,\vec{e}_\mu\vec{e}_{\mu'}\Theta^3_{\vec{r}_n}(\vec{r})\,\Theta^3_{\vec{r}_n\,'}(\vec{r}\,')\,\mathcal{C},\end{aligned}$$

where we calculate $\mathcal{C}$ explicitly

$$\begin{aligned}\mathcal{C} &= \hat{a}_{\mu,\vec{r}_n}\,\hat{a}_{\mu',\vec{r}_n\,'} + \hat{a}_{\mu,\vec{r}_n}\,\hat{a}^+_{\mu',\vec{r}_n\,'} - \hat{a}^+_{\mu,\vec{r}_n}\,\hat{a}_{\mu',\vec{r}_n\,'} - \hat{a}^+_{\mu,\vec{r}_n}\,\hat{a}^+_{\mu',\vec{r}_n\,'} \\ &\quad - \left(\hat{a}_{\mu',\vec{r}_n\,'}\,\hat{a}_{\mu,\vec{r}_n} + \hat{a}^+_{\mu',\vec{r}_n\,'}\,\hat{a}_{\mu,\vec{r}_n} - \hat{a}_{\mu',\vec{r}_n\,'}\,\hat{a}^+_{\mu,\vec{r}_n} - \hat{a}^+_{\mu',\vec{r}_n\,'}\,\hat{a}^+_{\mu,\vec{r}_n}\right) \\ &= \left[\hat{a}_{\mu,\vec{r}_n}, \hat{a}_{\mu',\vec{r}_n\,'}\right] + \left[\hat{a}_{\mu,\vec{r}_n}, \hat{a}^+_{\mu',\vec{r}_n\,'}\right] - \left[\hat{a}^+_{\mu,\vec{r}_n}, \hat{a}_{\mu',\vec{r}_n\,'}\right] - \left[\hat{a}^+_{\mu,\vec{r}_n}, \hat{a}^+_{\mu',\vec{r}_n\,'}\right].\end{aligned}$$

When we assume the desired commutation relations

$$\left[\hat{a}_{\mu,\vec{r}_n}, \hat{a}_{\mu',\vec{r}_n\,'}\right] = \left[\hat{a}^+_{\mu,\vec{r}_n}, \hat{a}^+_{\mu',\vec{r}_n\,'}\right] = 0 \tag{122}$$

$$\left[\hat{a}_{\mu,\vec{r}_n}, \hat{a}^+_{\mu',\vec{r}_n\,'}\right] = \delta_{\mu\mu'}\delta_{\vec{r}_n,\vec{r}'_n}, \tag{123}$$

the commutator becomes the original one in the continuous limit(119)

$$\begin{aligned}\left[\hat{E}_\mu(\vec{r}), \hat{A}_{\mu'}(\vec{r}\,')\right] &= \sum_{\vec{r}_n,\vec{r}'_n} \mathbf{i}\,\vec{e}_\mu\vec{e}_{\mu'}\Theta^3_{\vec{r}_n}(\vec{r})\,\Theta^3_{\vec{r}_n\,'}(\vec{r}\,') \underbrace{\left(\left[\hat{a}_{\mu,\vec{r}_n}, \hat{a}^+_{\mu,\vec{r}_n}\right] - \left[\hat{a}^+_{\mu,\vec{r}_n}, \hat{a}_{\mu,\vec{r}_n}\right]\right)}_{2\left[\hat{a}_{\mu,\vec{r}_n}, \hat{a}^+_{\mu',\vec{r}_n\,'}\right] = 2\delta_{\mu\mu'}\delta_{\vec{r}_n,\vec{r}'_n}} \\ &= 2\mathbf{i}\sum_{\vec{r}_n,\vec{r}'_n} \vec{e}_\mu\vec{e}_{\mu'}\delta_{\mu\mu'}\Theta^3_{\vec{r}_n}(\vec{r})\,\Theta^3_{\vec{r}_n\,'}(\vec{r}\,')\delta_{\vec{r}_n,\vec{r}'_n} \\ &= \mathbf{i}2\,\delta_{\mu\mu'}\sum_{\vec{r}_n}\Theta^3_{\vec{r}_n}(\vec{r})\,\Theta^3_{\vec{r}_n}(\vec{r}\,') \\ &\overset{\substack{\vec{L}\to\infty \\ \Delta_{r_i}\to 0}}{=} \mathbf{i}2\,\delta_{\mu\mu'}\delta(\vec{x}-\vec{x}\,').\end{aligned}$$

[63] See for example [Greiner et al., 2013, p. 78].

In fact, we see that the assumed discrete commutators (122) have the right continuous limit. Notably, the Bosonic commutation relations can only be fulfilled if at least one of both operators is unbounded. This was already proven during the beginnings of quantum mechanics by von Neumann v. Neumann [1931]. For the anti-commutator algebra of the Fermionic spinor operators this is not the case and hence the deduced commutation relations (120) are exact.

4.1.2 Discretized Operators

In this subsection, we deduce the general way to discretize operators that only depend on the fields. Operators with derivatives will be treated in the next section (4.2).

We construct the operators in our truncated Fock space by the "correspondence rules" of second quantization: given any $\hat{O}_H$ that acts on state vectors in a Hilbert space $|\psi\rangle$ and a Fock expansion $|\psi\rangle \to \hat{\psi}$, then the representation of $\hat{O}_F$ in the so constructed Fock space is given by[64]

$$\hat{O}_F = \int \hat{\psi}^+ \hat{O}_H \hat{\psi} \mathrm{d}^3 r. \tag{124}$$

As an illustration, we want to construct the Fock representation of the charge operator $\mathcal{C}$ with the expansion in rectangle functions

$$\hat{C}_F = \int \hat{\psi}^+ \, \hat{C}_H \, \hat{\psi} \mathrm{d}^3 r = \int \hat{\psi}^+ \left(e\underline{\beta}\right) \hat{\psi} \mathrm{d}^3 r \tag{125}$$

$$= e \sum_{\vec{r}_n, \vec{r}_n'} \underbrace{\sum_{\lambda,\lambda'} \vec{e}_\lambda \, \underline{\beta} \, \vec{e}_{\lambda'}}_{=(1,1,-1,-1)^T \equiv \vec{\beta}} \; \hat{c}^+_{\lambda,\vec{r}_n} \, \hat{c}_{\lambda',\vec{r}_n'} \underbrace{\int \Theta^3_{\vec{r}_n}(\vec{r}) \, \Theta^3_{\vec{r}_n\,'}(\vec{r}) \mathrm{d}^3 r}_{\delta_{\vec{r}_n \vec{r}_n\,'}} \tag{126}$$

$$\hat{C}_F = e \sum_{\vec{r}_n} \sum_{\lambda} \beta_\lambda \, \hat{c}^+_{\lambda,\vec{r}_n} \, \hat{c}_{\lambda,\vec{r}_n}. \tag{127}$$

This is enough to already find the expressions for the mass term

$$\hat{H}_{mass} = mc^2 \int_{\mathbb{R}^3} \mathrm{d}^3 r \, \frac{1}{2} \left[\hat{\psi}^+, \beta \, \hat{\psi}\right], \tag{128}$$

and the interaction term of the Hamiltonian

$$\hat{H}_{int} = -e \int_{\mathbb{R}^3} \mathrm{d}^3 r \, \frac{1}{2} \left[\hat{\psi}^+, \, \vec{\alpha} \cdot \hat{\vec{A}} \, \hat{\psi}\right]. \tag{129}$$

[64] A proof can be found for example in Gross et al. [1991].

4.2 Differential Operators in Finite Differences

In this section, we show how differential operators are constructed by means of the finite-differences method. Together with the contents of the last section, we are able to derive discretized differential operators. We demonstrate this explicitly for the kinetic energy operator. We want to mention at this point that the derivation is principally straight forward, but it becomes very technical. Therefore, the length of this chapter is rather short in comparison with the actual time and energy that were invested to get to the final form of the Hamiltonian.

Although the mode expansion discretizes the quantum fields, it is - in contrast to a continuous (complete) mode expansion - still not clear how differential operators act on these rectangle modes that are *not differentiable*.[65] The most common approach to do so is the finite-difference method (FD), that shall be discussed in this chapter.

In FD of n-th order a function f is interpolated by a polynomial $\mathcal{P}(n)$ of n-th order that is entirely defined through n given points $\{(p_i, f(p_i))|i = 1, \dots n\}$ of f. A differential operator $\mathcal{D}$ is then approximated as the derivative of $\mathcal{P}(n)$ at the points p_i. Consequently, it is a weighted difference expression between the p_i. It is possible to construct such an approximation coming from left, right or both sides, last of which is called central differences. For a second order approximation in central differences, the corresponding coefficients are given in table 2.[66]

Derivative	Accuracy	-1	0	1
1	2	$-1/2$	0	$1/2$
2	2	1	2	1

TAB. 2: Coefficients of the central finite differences method in second order. For example, the first derivative of a function f at the sampling point x_0 is approximated by $\partial_x f(x_0) = 1/\Delta_x(-1/2 f(x_{-1}) + 1/2 f(x_{+1})) + O(\Delta_x^3)$, where Δ_x denotes the spacing.

To apply the approximation on the rectangle discretization, we interpret the grid points as sampling points of the polynomials. This is done by the following replacement rules:

$$\partial_{r_i} \Theta_{r_{i,n}} = \frac{1}{2\Delta r_{i,n}} \left(\Theta_{r_{i,n+1}} - \Theta_{r_{i,n-1}} \right), \tag{130}$$

$$\partial^2_{r_i} \Theta_{r_{i,n}} = \frac{1}{(\Delta r_{i,n})^2} \left(\Theta_{r_{i,n+1}} + \Theta_{r_{i,n-1}} - 2\,\Theta_{r_{i,n}} \right). \tag{131}$$

To sum up, we want to bring the discretized kinetic energy operator as an example. The

[65] Actually one can define the derivative of a Θ function in a distributional sense, sloppy $\partial_x \Theta(x) = \delta(x)$. But this obviously would not make sense in our interpretation.

[66] Taken from Fornberg [1988].

kinetic energy operator is defined as

$$\hat{H}_{kin} = \int \hat{\psi}^{+} \hat{\mathcal{H}}_{kin} \hat{\psi} \mathrm{d}^3 r, \quad \hat{\mathcal{H}}_{kin} = -\mathbf{i}\, \underline{\vec{\alpha}} \cdot \nabla. \tag{132}$$

To construct its discretized version we identify its principal components

$$\hat{\mathcal{H}}_{kin} = -\mathbf{i}\hbar\, \hat{\psi}^{+}\, \underline{\alpha}_i\, \partial_i\, \hat{\psi} = \hat{\mathcal{H}}_{kin,x} + \hat{\mathcal{H}}_{kin,y} + \hat{\mathcal{H}}_{kin,z}.$$

As an example, we show

$$\begin{aligned}
\hat{\mathcal{H}}_{kin,x} &= -\mathbf{i}\hbar \sum_{\vec{r}_n, \vec{r}'_n} \underbrace{\sum_{\lambda,\lambda'} \hat{c}^{+}_{\lambda,\vec{r}_n}\, \vec{e}_\lambda\, \underline{\alpha_x}\, \vec{e}_{\lambda'}\, \hat{c}_{\lambda',\vec{r}'_n}}_{\equiv \mathcal{A}_x}\ \underbrace{\Theta^3_{\vec{r}_n}(\vec{r})\, \partial_x \Theta^3_{\vec{r}_n\,'}(\vec{r})}_{\equiv T_x} \\
&\to \int \mathrm{d}^3 r T_x = \frac{1}{2\Delta_x} \left(\delta_{x_n x'_{n+1}} \delta_{y_n y'_n} \delta_{z_n z'_n} - \delta_{x_n x'_{n-1}} \delta_{y_n y'_n} \delta_{z_n z'_n} \right) \\
&\to \mathcal{A}_x = e_1\, \delta_{\lambda 1} \delta_{\lambda' 4} + e_2\, \delta_{\lambda 2} \delta_{\lambda' 3} + e_3\, \delta_{\lambda 3} \delta_{\lambda' 2} + e_2\, \delta_{\lambda 4} \delta_{\lambda' 1} \\
&\equiv \sum_{\lambda} \hat{\mathcal{H}}_{kin,x,\lambda}.
\end{aligned}$$

From these 4 terms, the first is:

$$\hat{H}_{kin,x,1} = -\frac{\mathbf{i}\hbar}{2\Delta_x} \sum_{\vec{r}_n} \left(\hat{c}^{+}_{1,\vec{r}_n} \hat{c}_{4,x_{n+1} y_n z_n} - \hat{c}^{+}_{1,\vec{r}_n} \hat{c}_{4,x_{n-1} y_n z_n} \right)$$

The other terms are computed by a change of indices according to $\mathcal{A}_x$. For the x and y component the delta symbols are listed, respectively:

$$\begin{aligned}
\int \mathrm{d}^3 r T_y &= \frac{1}{2\Delta y} \left(\delta_{x_n x'_n} \delta_{y_n y'_{n+1}} \delta_{z_n z'_n} - \delta_{x_n x'_n} \delta_{y_n y'_{n-1}} \delta_{z_n z'_n} \right) \\
\mathcal{A}_y &= e_1\, \delta_{\lambda 1} \delta_{\lambda' 4} + e_2\, \delta_{\lambda 2} \delta_{\lambda' 3} - e_3\, \delta_{\lambda 3} \delta_{\lambda' 2} - e_4\, \delta_{\lambda 4} \delta_{\lambda' 1} \\
\int \mathrm{d}^3 r T_z &= \frac{\mathbf{i}}{2\Delta z} \left(\delta_{x_n x'_n} \delta_{y_n y'_n} \delta_{z_n z'_{n+1}} - \delta_{x_n x'_n} \delta_{y_n y'_n} \delta_{z_n z'_{n-1}} \right) \\
\mathcal{A}_z &= e_1\, \delta_{\lambda 1} \delta_{\lambda' 3} + e_2\, \delta_{\lambda 2} \delta_{\lambda' 4} + e_3\, \delta_{\lambda 3} \delta_{\lambda' 1} + e_4\, \delta_{\lambda 4} \delta_{\lambda' 2}
\end{aligned}$$

Also the electromagnetic part of the Hamiltonian

$$\hat{H}_{em} = \frac{\epsilon_0}{2} \int_{\mathbb{R}^3} \mathrm{d}^3 r \left(\left(\nabla \times \hat{\vec{A}} \right)^2 + \left(c \hat{\vec{E}} \right)^2 \right) \tag{133}$$

can now be treated. The derivation of the whole Hamiltonian in its discretized form is given in Appendix A.1.

Crucially, these results shed light on a disadvantage of the real-space picture: it does not belong to eigenstates of the free theories, so the mode expanded Hamiltonian has many

terms.

4.3 Numerical Implementation

The approach introduced in the last sections is very well suited for numerical studies. We do this in a Matlab code that works directly on the operator level. For that, we derive in the first subsection (4.3.1) creation and annihilation (C/A) operators that act in the truncated Fock space. Therefore, we do not have to implement the underlying n-particle states. This results in a framework that allows for exploring the *complete* Fock space of the (truncated) problem. We show the results in the next chapter 5.

In the second subsection 4.3.2, we explain how we derived our model system, that for computational capacity reasons is very low-dimensional. The full Hamiltonian can be found in the Appendix A.3.

4.3.1 Matrix Representation of Creation and Annihilation Operators

In the truncated Fock space, all operators can be represented by finite matrices. To keep things simple we show their form for a linear chain of N sites with maximal B Bosonic levels per site. This can of course be expanded trivially to a full 3D model. The matrix that creates/destroys a Boson on site i can be constructed by the algebra of the creation/annihilation (C/A) operators

$$\begin{aligned} \hat{a}_i^+ \left|n_0, n_1, \ldots, n_i, \ldots, n_N\right\rangle_B &= \sqrt{n_i + 1}\left|n_0, n_1, \ldots, n_i + 1, \ldots, n_N\right\rangle_B \\ \hat{a}_i \left|n_0, n_1, \ldots, n_i, \ldots, n_N\right\rangle_B &= \sqrt{n_i}\left|n_0, n_1, \ldots, n_i - 1, \ldots, n_N\right\rangle_B . \end{aligned} \tag{134}$$

We choose the set of all Bosonic number states

$$\left|n_0, n_1, \ldots, n_N\right\rangle_B \rightarrow \vec{n}_0 \otimes \vec{n}_1 \otimes \cdots \otimes \vec{n}_N \tag{135}$$

as basis, where we write the $\vec{n}_i$ as column vectors

$$\vec{n}_i = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ B \end{pmatrix} \quad i = 1, 2, \ldots, N. \tag{136}$$

The vectors hence are B^N-dimensional. For any site the respective creator/annihilator is a $B \times B$ matrix[67]

$$\hat{a}^+ = \begin{pmatrix} 0 & \sqrt{1} & 0 & \cdots & 0 \\ 0 & 0 & \sqrt{2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \sqrt{B} \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{137}$$

$$\hat{a} = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ \sqrt{0} & 0 & 0 & \cdots & 0 \\ 0 & \sqrt{1} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \sqrt{B-1} & 0 \end{pmatrix} \tag{138}$$

and the complete $B^N \times B^N$ matrix that acts on (135) is given by the Kronecker product between those and several $B \times B$ identity matrices $\mathbb{1}_B$

$$\hat{a}_i^+ = \underbrace{\mathbb{1}_B \otimes \cdots \otimes \mathbb{1}_B}_{(i-1)-\text{times}} \otimes \hat{a}^+ \otimes \underbrace{\mathbb{1}_B \otimes \cdots \otimes \mathbb{1}_B}_{(N-i)-\text{times}}. \tag{139}$$

These operators obey the Bosonic commutation relations except for a truncation error

$$\left[\hat{a}_i, \hat{a}_j^+\right] = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1-B \end{pmatrix}. \tag{140}$$

This error plays an important role during the exploration of the Fock space and is discussed in section 7.2.

For the Fermionic C/A operators we do the same without the necessity of truncating any levels because the Pauli principle already reduces them to two. In exchange we need to explicitly introduce anti-symmetry in the representation, to have anti-commutators between all sites. This is done through the *Jordan-Wigner Transformation* [Jordan and Wigner, 1993]. We describe the Fermionic state for a field with two spin components[68] in analogy to having twice as many sites

$$\left|n_{0,\uparrow}, n_{0,\downarrow}, \ldots, n_{N,\uparrow}, n_{N,\downarrow}\right\rangle_F \equiv \left|n_1, n_2, \ldots, n_{2N}\right\rangle_F \tag{141}$$

[67] We identify here and in the following the matrix representation $\hat{a}_M$ with the abstract $\hat{a}$ and drop the index M to keep the number of indices low.

[68] For QED this would be 4 for all the 4 components fo the Dirac spinor.

which are formed by a Kronecker product of column vectors

$$|n_1, n_2, \ldots, n_{2N}\rangle_F \rightarrow \vec{n}_0 \otimes \vec{n}_1 \otimes \cdots \otimes \vec{n}_{2N},$$
$$\vec{n}_i = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad i = 1, 2, \ldots, N. \tag{142}$$

Then the creation/annihilation matrices on any site are just the circular Pauli matrices

$$\hat{c}^+ = \sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{c} = \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{143}$$

The Jordan-Wigner transformation now tells us that for the respective matrix of the whole Fermionic Fock space, we must include the third Pauli matrix

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{144}$$

in the following way:

$$\hat{c}_i^+ = \underbrace{\mathbb{1}_2 \otimes \cdots \otimes \mathbb{1}_2}_{i-1 \text{ times}} \otimes \sigma^+ \underbrace{\otimes \sigma_z \otimes \cdots \otimes \sigma_z}_{2N-i \text{ times}} \tag{145}$$

Through such a construction the Fermionic anti-commutation rules

$$[c_i, c_j^+]_+ = \delta_{ij} \tag{146}$$

are satisfied over the whole grid. Finally the operators of the coupled space of Bosons and Fermions are easily found as the Kronecker products

$$\hat{a}_{i,\text{coupled}}^{(+)} = \hat{a}_i^{(+)} \otimes \underbrace{\mathbb{1}_2 \otimes \cdots \otimes \mathbb{1}_2}_{2N \text{ times}} \tag{147}$$

$$\hat{c}_{i,\text{coupled}}^{(+)} = \underbrace{\mathbb{1}_B \otimes \cdots \otimes \mathbb{1}_2}_{N \text{ times}} \otimes \hat{c}_i^{(+)} \tag{148}$$

because both spaces are disjoint. Throughout the following chapters, we only use these operators and hence drop the "coupled" indication.

4.3.2 The Model System: A 2-Site-1-Mode-Hamiltonian

The biggest advantage of our approach that allows for to investigating the whole Fock space of a QED system coincides with its biggest disadvantage: Its degrees of freedom grow extremely fast with the dimension of the system. If we have N sites and B Bosonic

levels the dimension of the Fock space becomes

$$F = (4^2)^N * B^N. \tag{149}$$

Only to describe the smallest possible motion in three directions ($N = 8$ points), and allow for the minimal Bosonic dynamics with $B = 2$ Bosonic levels, equation (149) results in $F \approx 10^{12}$. Hence, the state vectors would be $F \approx 10^{12}$-dimensional and the corresponding matrices could not even be diagonalized on a huge cluster.

Nevertheless we can do very general research about the Fock space in terms of symmetries and limits to other theories. For that we derived something like the minimal model of our QED Hamiltonian, which describes the dynamics of a full Dirac spinor that is strongly confined in two directions and very poorly resolved in the third one by two sites. It interacts with Maxwell Bosons that are as confined as the Fermions, so that only one mode with two degrees of freedom is considered. The derivation of the corresponding Hamiltonian can be found in Appendix A.3.

5 Numerical Results for Finite Differences

With the help of the model developed in last chapter, we shall now show the first results for the finite-differences (FD) discretization in this chapter. To explore the complete Fock space, our technique of choice is exact diagonalization (ED). To keep things as simple as possible, we restrict ourselves to time-independent phenomena in this work. Yet, we could include time evolution with, for example, the Lanczos algorithm [Lanczos, 1950].

In the first section (5.1), we introduce the important numerical parameters and have a look into the structure of the Hamiltonian to get a feeling for the formalism. In the second section (5.2), we show how to make use of the possibility to control the parameters of the theory and we investigate limits to other theories. We conclude in section 5.2 by analyzing the symmetry structure of the theory.

5.1 Exact Diagonalization for Finite-Differences

As mentioned in subsection 4.3.2, the dimensionality of the problem rises extremely fast. Hence, we are limited to a Hamiltonian for N=2 sites and B=2 Bosonic degrees of freedom to still be able to perform numerical studies. The corresponding state vectors have according to (149) the dimension

$$F = (4^2)^N * B^N \quad \overset{\substack{N=2\\ \rightarrow \\ B=2}}{} \quad F = (4^2)^2 * 2^2 = 1024$$

and hence the Hamiltonian H is a (1024×1024)-matrix. Throughout this chapter all figures respect those parameters, when not indicated otherwise.

For the finite-differences method, there is the possibility to include different types of boundary conditions.[69] If not indicated differently, in this chapter these are of Dirichlet-type, which physically corresponds to a resonator. Explicitly, for any operator $\hat{b}$, we have

$$\hat{b}(0) = \hat{b}(N+1) = 0. \tag{150}$$

Additionally, we can impose periodic boundary conditions (PBC)

$$\hat{b}(1) = \hat{b}(N+1). \tag{151}$$

These are imposed in chapter 7 for a better comparison to the Fourier method that is introduced in chapter 6.

We want to mention that all calculations are performed in atomic units (a.u.), which

[69] In contrast to the Fourier method, that is presented in chapter 6

Dimension	Expression	Value in SI-units
mass	m_e	$9.10938291(40) \cdot 10^{-31} kg$
charge	e	$1.602176565(35) \cdot 10^{-19} C$
action	$\hbar$	$1.054571726(47) \cdot 10^{-34} Js$
length	$a_0 = \hbar/(m_e c\alpha)$ (Bohr)	$5.2917721092(17) 10^{-11} m$
energy	$E_h = \alpha^2 m_e c^2$ (Hartree)	$4.35974417(75) 10^{-18} J (= 27,2eV)$

TAB. 3: Overview over the most important quantities in atomic units.[70]

are appropriate for atomic scales. We obtain them by setting the electron mass m_e, the elementary charge e, Planck's constant $\hbar$ and the Coulomb force constant $1/(4\pi\epsilon_0)$ to one. The speed of light becomes $c = 1/\alpha \approx 137$, with the fine-structure constant $\alpha \approx 1/137$, that being dimensionless has the same value in every unit system. The derived units are given in table 3.

Let us now turn to the Hamiltonian. In figure 6, we show the so-called *sparsity pattern* of H, which shows all entries in H that are not zero, and its eigenvalues. We see that most of the entries are zero and it has a symmetric structure. The eigenvalues of H are (nearly) symmetrically distributed around zero and there are

$$L = 4N + 1 = 9 \tag{152}$$

main energy manifolds, which for our case of $N = 2$ yields $L = 9$. These are the main Fermionic energy levels. We can understand this number by a qualitative view on the total charge operator C. We know from the continuous case that it counts two entries of the spinor negative and two entries positive and so justifies the particle/antiparticle-interpretation. Hence, every site can maximally have total charge $C_{max} = 2$ and minimally $C_{min} = -2$, so summed up for N sites we have

$$C_{N,max} = 2N, \quad C_{N,min} = -2N. \tag{153}$$

As all the intermediate values are also possible, we find (152). In the regime that we analyze here, these charge energies are dominating over all others and so we see the $L = 9$ manifolds. We do not want to get into further detail on the various operators and their properties here, but leave this discussion for the following sections. We just want to emphasize that the form of L is especially due to the combinatorics problems of how many options there are to distribute particles in the system. Therefore, also other operators exhibit the same number of eigenvalue manifolds (like the momentum term of the Hamiltonian, see 7).

[70] SI units are taken from The NIST Reference on Constants, Units, and Uncertainty 2016, see http://physics.nist.gov/cuu/Constants/index.html.

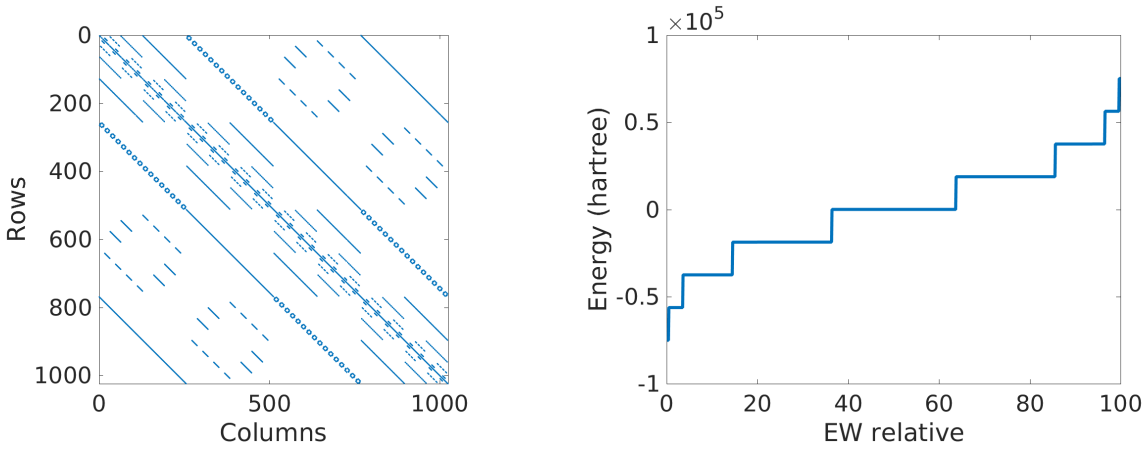

FIG. 6: The sparsity pattern of the Hamiltonian (left) and its eigenvalues (right).

In the next figure (7), we show the individual parts of the Hamiltonian, which show that the manifolds are not entirely degenerated. There are small deviations on different scales present and the electromagnetic term introduces a small asymmetry of the spectrum. We discuss the contributions of the individual terms of the Hamiltonian later in section 7.1.

At this point, we want to emphasize that all comparisons between *different* parameter choices that we perform in the following, have to be treated carefully. To make robust statements, we would need to implement a proper renormalization technique, like for example in the approach of R. Grobe (see subsection 2.2.4). This will hopefully be the topic of a subsequent work. A good starting point is our possibility to compare two different methods of discretization with actually very strong deviations in certain regimes. This is discussed in section 7.1.

Nevertheless, the found eigenvalue structure fits well to the typical interpretation of QED: the positive (negative) energies correspond to eigenstates with a surplus of electrons (positrons), the electromagnetic interaction splits the main electronic energy manifolds and shifts them slightly to more negative energies as the interaction term enters negative in the Hamiltonian.[71]

[71] The Hamiltonian exhibits negative eigenvalues because we did not perform a renormalization procedure like that mentioned in subsection 3.2.1. This will be part of future work.

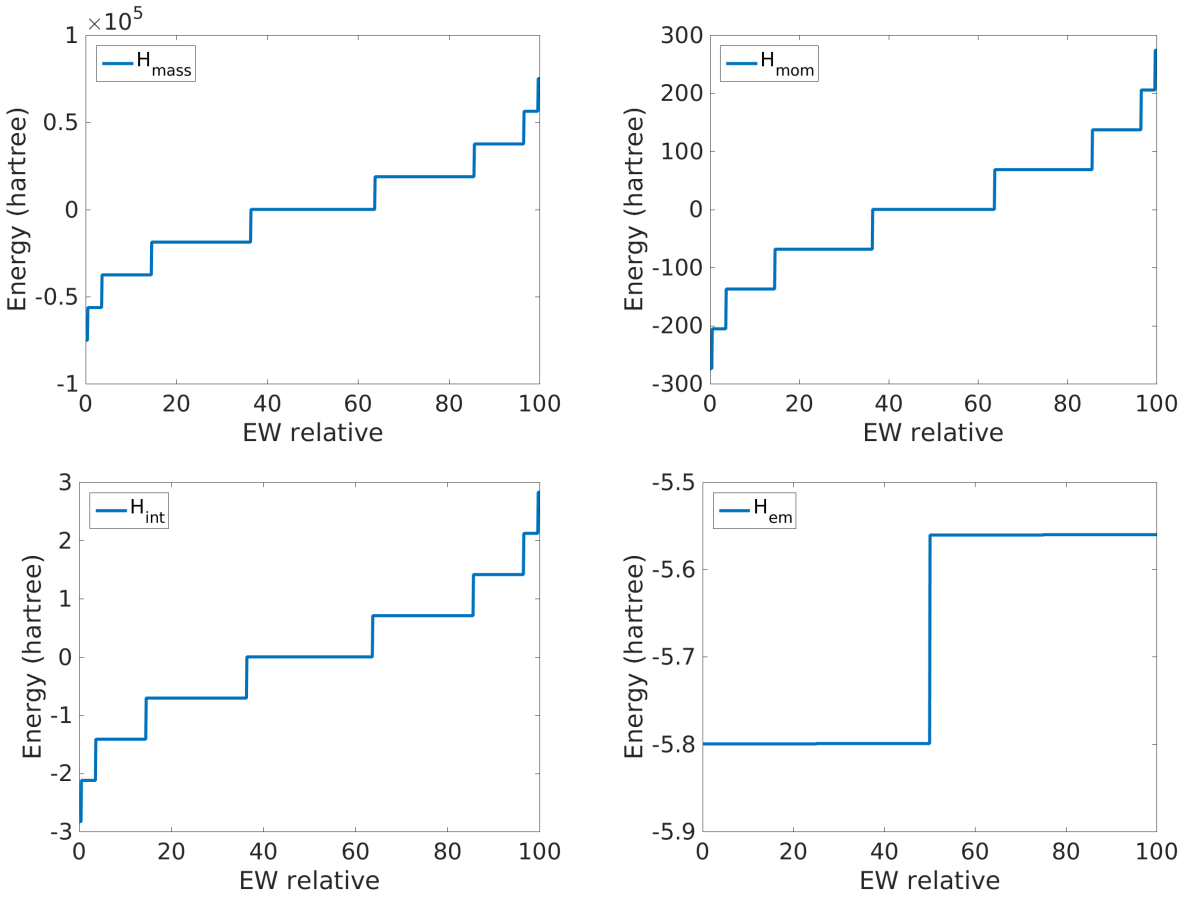

FIG. 7: Contribution of the different constituents to the energy spectrum of the Hamiltonian: the mass-term (up, left) dominates with energy scales around 10^4 Hartree, followed by the momentum term (up, right) with energy contributions of up to 300 Hartree. The smallest contributions are due to the interaction (down, left) and the electromagnetic term (down, right). All terms are symmetric around zero energy, except the electromagnetic term. It only contributes negative energy.

5.2 Lattice QED under Variation of Parameters

In this section we investigate the influence of the parameters of the theory on the energy spectrum of the Hamiltonian H. This allows us to visualize the transition of QED to certain limit cases, that are

1. the non-relativistic limit: $c \to \infty$[72],
2. the strong coupling limit: $e \to \infty$

and we can investigate the dependence of H in terms of

3. the mass m of the QED electrons and
4. the influence of the spacing Δ_x.

The last case is unfortunately not separable from the confinement $L = N \cdot \Delta_x$, because we cannot increase the number of grip points N for computational reasons. We want to emphasize that the following calculations are not exhaustive investigations about limits or renormalization, they should rather be considered as "proofs of principles." There is still a lot of potential in these limits like comparisons to the analytically derived limits, that we want to explore in future research. The interested reader is referred to the outlook, chapter 9.

1. Variation of c

   In figure 8, the variation of the speed of light, c, is depicted. With increasing c, we see that the energy levels rapidly approach each other until they are (nearly) completely degenerated to the already discussed $L = 4N + 1 = 9$ equidistant manifolds. The high-c regime (down, right) strongly suggests that the degeneration becomes complete for $c \to \infty$. This is also predicted by analytical studies (see Bialynicki-Birula and Bialynicka-Birula [1984]). Numerically, this corresponds to the domination of the rest-energy, because all other terms have a weaker c-dependence and hence become negligible for a high c-value. Hence, we can interpret this as the expected decoupling between electron and positrons in the non-relativistic limit, where the Pauli-equation describes pure electrons (or positrons) with their spin Bialynicki-Birula and Bialynicka-Birula [1984].

   For small c-values instead, we see that the already recognized asymmetry between negative and positive energies becomes stronger. This is the opposite effect: the

[72] As c is connected to the electric and magnetic constants ϵ_0, μ_0 through the dispersion relation $1/c^2 = \epsilon_0\mu_0$, there are actually different non-relativistic limits. This shall not be further discussed here and the reader is referred to Le Bellac and Lévy-Leblond [1973]

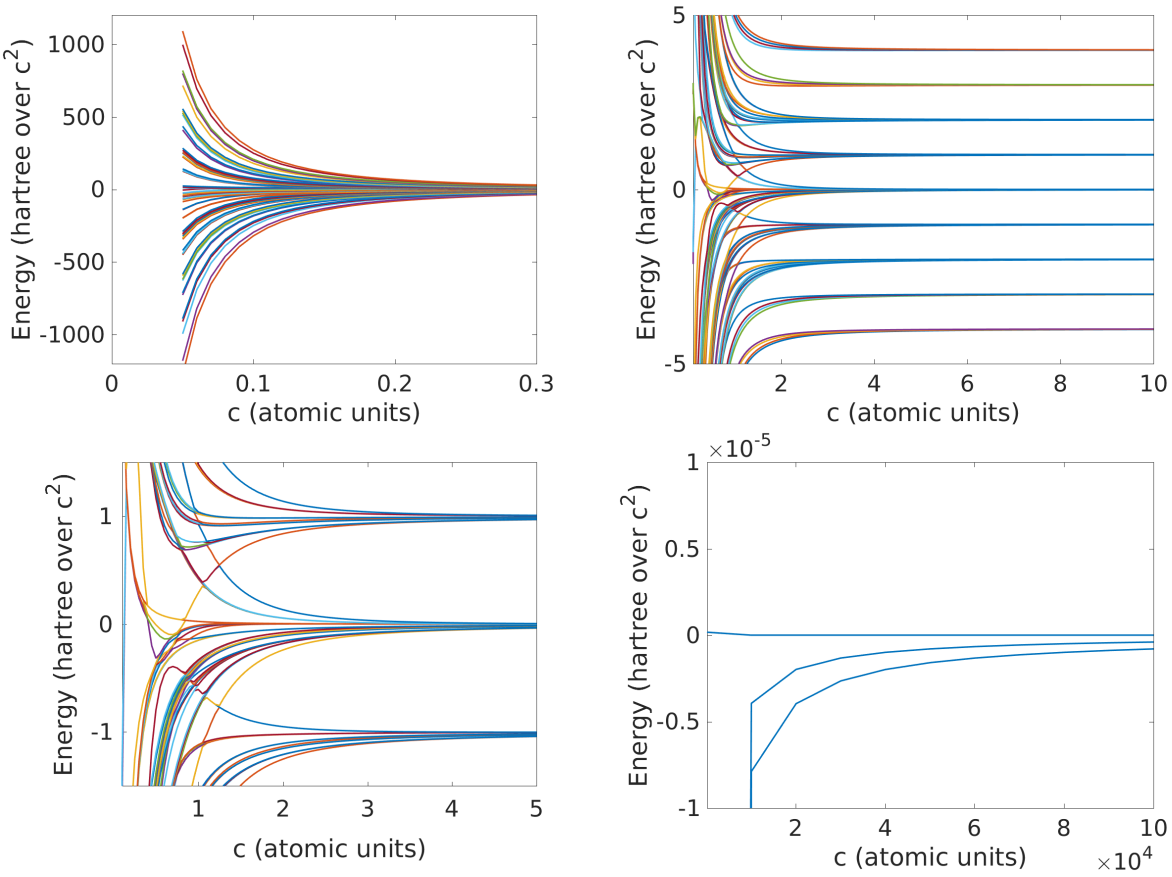

FIG. 8: Energy spectrum of H (normalized to the rest energy of an electron $m_e c^2$) as a function of the velocity of light c for different scales: We see the general trend of all eigenvalues degenerating in the up-left figure. The up-right figure shows that 9 energy manifolds remain in the non-relativistic limit. Every energy manifold has contributions from the whole spectrum, so energy levels cross each other (down-left figure) and for very high c, the levels approach each other very close (down-right figure). Notably, the colors do not correspond to one certain state but rather to one entry in the array of eigenvalues that is sorted.

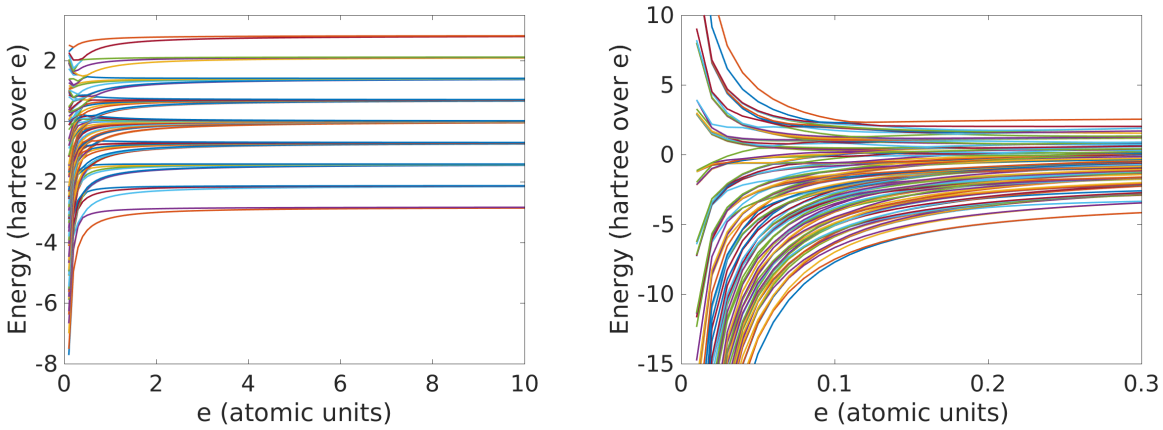

FIG. 9: Energy spectrum of H as a function of the charge e (normalized by e): We see that the energy levels degenerate very fast to the 9 decoupled manifolds (left). We see that the process of degeneration is different compared to the variation of c, but there are still line-crossings present (right).

energy is especially dominated by the interaction and the magnetic term that do not depend on c.

The comparison of figure 8 to figure 6 from the last subsection, where the "real" $c = 137$ in atomic units was chosen, shows that these "real" units correspond to a very non-relativistic regime in our model. This is because the resonator with $L = 2 * \Delta_x = 2a_0$ is on the scale of small atoms and so very large with respect to relativistic scales. In the following, we distinguish between the relativistic and non-relativistic regime through the artificial change of c. The influence of the box is instead analyzed later in this section (see figure 11).

2. Variation of e
   The results of the variation of the electric charge e (, which is the coupling constant between Fermions and Bosons) are shown in figure 9. The calculations were performed in the relativistic regime by setting $c = 0.1$, to analyze the non-degenerate spectrum. We see that the spectrum degenerates comparably to the non-relativistic limit.[73] We did not show the relativistic case, where we already have the degenerate spectrum for small e and where these just stay degenerate. But here this is not due to the electron-positron decoupling but the opposite: the Fermions are maximally coherent and they act again like free particles. This was for example already observed in the non-relativistic case Pellegrini et al. [2015].

3. Variation of m
   We show the variation of the electron mass m_e in figure 10. Our analysis was performed in the relativistic regime by setting $c = 0.1$ in order to investigate the

[73] We also calculated the spectrum for very high e and confirmed that they approach each other to (arbitrary) small distances.

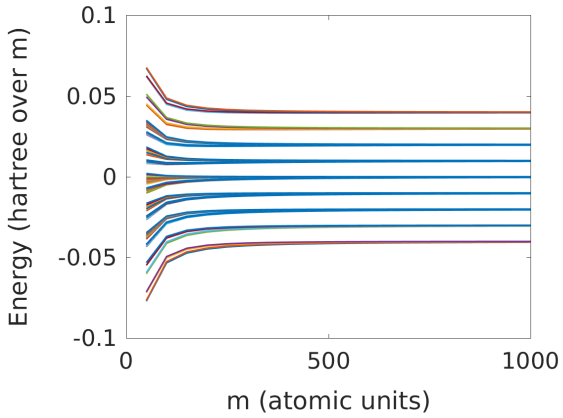

FIG. 10: Energy spectrum of the Hamiltonian as a function of the electron mass m (normalized by m): We see like in the other cases that the energy levels degenerate very fast to the 9 decoupled manifolds.

non-degenerate spectrum. We see that the spectrum degenerates similarly to the non-relativistic and the strong coupling limit, so we have free particles. This is also explainable as the interaction becomes unimportant for very heavy particles.

4. Variation of Δ_x
   Eventually, the results of the variation of the spacing Δ_x is depicted in figure 11. Here, we did not change any other constant. As Δ_x is strongly connected to the ultraviolet divergence of QED, we can assume that results for different Δ_x cannot be compared well. We would need to apply a renormalization technique. However, the Grobe group found in their approach a logarithmic divergences for the energy Wagner et al. [2013]. Therefore, we plotted all data with logarithmic Δ_x axis, although we can guess that this is not enough to have reasonable energies values.

   In the plot, we can see how the degeneracies are lifted for a small resonator length $L = \Delta_x \cdot N$. The nine manifolds split into four strands, that by themselves consist of 9 energy manifolds. These manifolds are probably related to the formation of standing waves in the small resonator. Unfortunately, we could not investigate this deeper as we are not able to increase the number of grid points so far.

   Later in section 7.1, we will again look at the variation of Δ_x, because finite-differences and the Fourier method (introduced in chapter 6) depend differently on Δ_x.

5.3 Symmetries in Finite-Differences

In this section, we analyze the symmetry aspects of the finite-difference Hamiltonian. Later, we compare this to the Fourier method (section 7.2).

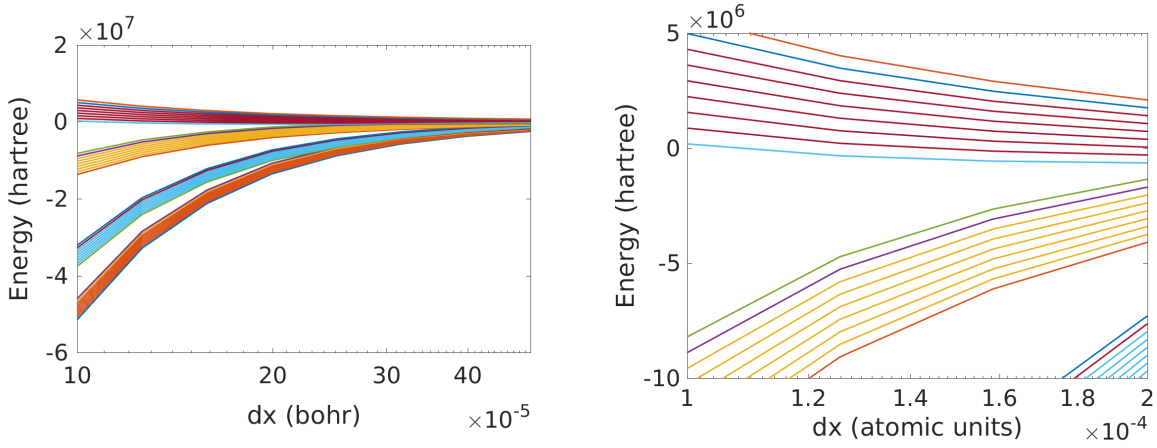

FIG. 11: Energy spectrum of the Hamiltonian as a function of the (logarithmic) spacing Δ_x (*not* normalized and denoted by dx in the plot): On the left, we can see how the lifting of degeneracy takes places for small spacing and consequently small resonator length $L = \Delta_x \cdot N$. The 9 energy manifolds split into four strands, that by themselves consist of 9 manifolds (with lower degree of degeneracy). This can be seen well in the right plot.

We want to study the behavior of the Hamiltonian H under symmetry transformations. From the theoretic considerations in section 2.3, we know that symmetries of H should block-diagonalize it. Therefore, let us assume an operator O[74] with eigenvectors $|\Psi_l\rangle$ and corresponding eigenvalues o_l

$$O\,|\Psi_l\rangle = o_l\,|\Psi_l\rangle\,, \tag{154}$$

that commutes with H

$$[O, H] = 0. \tag{155}$$

Then the $|\Psi_l\rangle$ combined to a matrix form a unitary transformation

$$U = (|\Psi_1\rangle\,, |\Psi_2\rangle\,, \ldots |\Psi_F\rangle) \tag{156}$$

that brings H in block-form, where the blocks are labeled by the eigenvalues o_l.

All possible symmetries of QED are known (see chapter 2.3). There are the discrete charge conjugation, parity and time reversal symmetries that we have not analyzed in this work. It may be part of future investigations. Then, there is local gauge invariance that we definitely loose in our discretized theory.[75] Nevertheless, the global gauge symmetry and, corresponding to that, charge is preserved. We analyze this in the first subsection (5.3.1) together with the behavior of the particle number operator. Due to pair-creation and -annihilation processes in QED, the particle number should not be conserved in contrast to non-relativistic theories. However, we find it being conserved and the reasons are still

[74] We drop the hat symbol in this section, since it is clear that operators are meant.
[75] As discussed in the introduction to chapter 4.

unclear.

Lastly, there are the Poincaré symmetries, that consist of a pure local part, the Lorentz transformations, and a translation part. From those, only translational invariance can be approximated well by a space(-time) lattice. This will be the content of the second section 5.4.

We do not further analyze Lorentz transformations, but we want to remark that indeed it is possible to construct a grid, that exhibits a discrete form of rotational invariance.[76] We mean this in the sense, that we can approximate the rotation angle with arbitrary precision. We can for example just choose polar coordinates and discretize those in the same way as the Cartesian ones. But this always needs a symmetry axis (the center of rotation) which distinguishes one point of the grid. Consequently, it is only possible to describe a *global* Lorentz invariance well, which is simply the case, when the boundary conditions have that symmetry. The local Lorentz invariance of every grid point can only be approximated with one definite angle for every grid structure. Thus, there is no possibility of sampling such rotations finer. A 2D quadratic grid for example exhibits only invariance under 4 rotations. In contrast to that, we can render the minimal distance between translations arbitrarily small. In section 6.3, this is also discussed by means of the Fourier method.

5.3.1 Total Charge and Particle Number

We first want to analyze operators, that are not influenced by the discretization method. The first example is the total charge operator that is related to global gauge invariance

$$\hat{C} = e \int \mathrm{d}^3 r \hat{\psi}^+ \hat{\psi}. \tag{157}$$

This definition has to be slightly modified to get the right spectrum of the eigenvalues. This is due to the interpretation of the $\hat{\psi}$-operator. To get negative and positive eigenvalues, we need to introduce the positron picture as shown in subsection 3.2.1:[77]We reinterpret the third and fourth component of $\hat{\psi}$ so that the role of the creation and annihilation operators are exchanged.

In figure 12 we can see how the total charge eigenvalues label the blocks in the spectrum of H. Every block by itself contains a symmetric spectrum of positive and negative values. For example, if we want to describe a physical situation with a total charge of zero, only 256 of the 1024 eigenvalues of the Hamiltonian are important for any dynamics. Hence, we only need to diagonalize 256×256-matrices and save computational costs up to a

[76] The Lorentz group is the double cover of the group of complex rotations SU(2).

[77] In the subsection, this is shown for momentum modes, but it is a general phenomenon. A general definition of positron operators is given in Bialynicki-Birula and Bialynicka-Birula [1984].

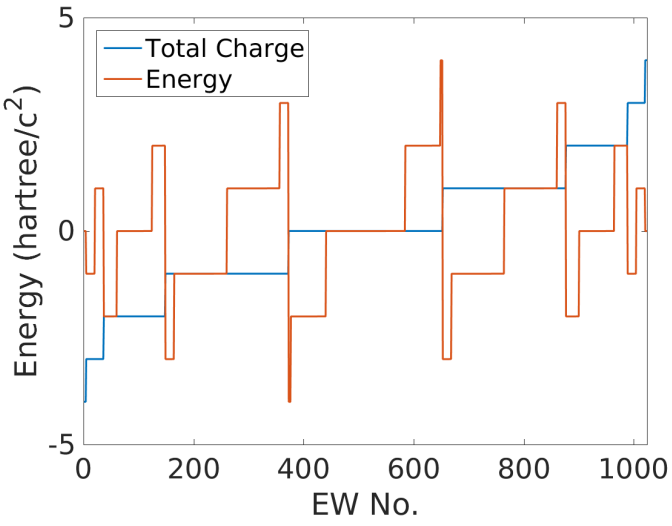

FIG. 12: Energy spectrum of the Hamiltonian that is block-diagonalized through the total charge operator: There are nine blocks that correspond to the nine different charge eigenvalues.

factor of $4^3 = 64$.[78]

The second example is the Fermion number operator

$$\hat{N} = \int \mathrm{d}^3 r \, \hat{\psi}^+ \underline{\beta} \hat{\psi}. \tag{158}$$

In QED, this actually should not be a symmetry, because photons can spontaneously create electron-positron pairs. Interestingly, our finite differences Hamiltonian H actually *commutes* with N. We still do not exactly know why this is, but it is probably related to the particle/antiparticle interpretation. This will be part of future research.

5.4 Translational Invariance

In this last section for the finite-differences method, we want to discuss the invariance of the theory under translations. The Hamiltonian H is invariant under translations, if it commutes with the corresponding generator, the generalized momentum operator

$$\hat{\vec{P}} = \int \mathrm{d}^3 r \hat{\psi}^+ \left(-\mathbf{i}\hbar\nabla - e\hat{\vec{A}} \right) \hat{\psi}. \tag{159}$$

In our matrix-based code, we can easily implement such a commutator. The problem of the full $\hat{\vec{P}}$ is, that it contains Bosonic operators, that by definition have a commutation error (see subsection 4.3.1). Together with the Fourier method, this is discussed in section 7.2. Hence, we only consider here the bare Dirac theory excluding Bosonic operators. The

[78] The numerical diagonalization of a $N \times N$-matrix scales with N^3. See Golub and Van Loan [1996].

respective momentum operator is

$$\hat{\vec{P}}_{Dirac} = -\mathbf{i}\hbar \int \mathrm{d}^3 r \psi^+ \nabla \psi. \tag{160}$$

We found as expected that $\hat{\vec{P}}_{Dirac}$ commutes with $\hat{H}_{Dirac}$, although we cannot block-diagonalize $\hat{H}_{Dirac}$ explicitly. This is due to numerical problems with pure imaginary, but symmetric entries. The corresponding eigenvalues are purely real-valued. Consequently, they are computed by sums of complex conjugated pairs. This is numerically very unstable, because little deviations in the imaginary parts between two theoretically complex conjugated numbers lead to imaginary rests in their sum.

6 Group Theoretical Approach

In this chapter, we derive a second method, besides finite-differences, to discretize the differential operators of our theory. This will be done by means of representation theory of the symmetry group of a discrete lattice.

We begin in the first section 6.1 by inquiring the coordinate space to be discrete, which is the most fundamental postulate in a group-theoretical perspective. We introduce a 3D Cartesian grid to develop our Hamiltonian theory. This somehow samples a possible spatial part of the Minkowski space. The grid has discrete translational symmetry and is invariant under a four element rotation group. We do not discuss the time degree of freedom and so also for example no Lorentz-boosts. Then, we need to define the state space. The entries of the spinor waves are functions over the coordinate space. In the continuous theory, the correspondence would be a Hilbert space. We define such a "finite Hilbert space" as the space of bounded discrete functions with a proper inner product.

In the next and main section (6.2), we introduce translations and their generator, the momentum operator. Within the framework presented in the first section, we show a general rule to derive representations of differential operators of any order. Moreover, we show how differential operators they act on a choice of model state functions and we compare the method to finite differences. Lastly, we also define the position operator. With the position operator, we are able to analyze the fundamental commutation relations of the finite theory.

In section 6.3, we briefly discuss the other symmetry operators, which may be of importance for future work.

6.1 The Framework: A Discrete World

In this section, we introduce the relevant setting for our group theoretical approach.

Let us define a 3D bounded discrete space L, formally with spacing Δ[79]

$$L = (\{1, 2, \ldots, N\} * \Delta)^3. \tag{161}$$

These 3N grid points are meant to sample a compact subset of the continuous real space $K \subset \mathbb{R}^3$. This could be a cuboid or a ball in the spatial Minkowski space.

On L, we now need to define how to "sample" the state space, which is a vector space and with inner product. Hence, we want to define the vector space of all bounded complex

[79] To keep things simple, we assume the same spacing in all three dimensions: $\Delta_x = \Delta_y = \Delta_z = \Delta$.

valued functions over L

$$\begin{aligned} &f \in \mathcal{C}[L] = \{f : L \to \mathbb{C} | \|f\| < \infty\} \\ &f : L \to \mathbb{C}, \quad f(\vec{x}) \equiv f_{\vec{x}} \equiv f_{x_1,x_2,x_3} \in \mathbb{C}, \quad i,j,k \in L. \end{aligned} \tag{162}$$

with the *inner product*

$$\begin{aligned} &\langle \cdot \,|\, \cdot \rangle : \mathcal{C}[L] \times \mathcal{C}[L] \to \mathbb{C}, \\ &\langle f \,|\, g \rangle = \sum_{\vec{x}=1}^{N} f^*_{\vec{x}}\, g_{\vec{x}} \in \mathbb{C} \qquad \text{for } f,g \in \mathcal{C}[L]. \end{aligned} \tag{163}$$

and the corresponding norm

$$\|\cdot\| : \mathcal{C}[L] \to \mathbb{C}, \tag{164}$$

$$\|f\| = \sqrt{\langle f \,|\, f \rangle} \in \mathbb{C} \qquad \text{for } f \in \mathcal{C}[L]. \tag{165}$$

The theory converges for $N \to \infty$ to the continuum limit $\mathcal{H}[K]$. It is the space of square-integrabel functions $L[K \in \mathbb{R}^3]$ with inner product

$$\langle f \,|\, g \rangle = \int_K f^*(\vec{x})\, g(\vec{x})\, \mathrm{d}^3 r \qquad \text{for } f,g \in \mathcal{H}[K]. \tag{166}$$

At this point, we are able to define *unitary transformations U*. They are linear maps that leave the inner product invariant

$$U : \mathcal{F}[L] \to \mathcal{F}[L], \tag{167}$$

$$\langle Uf \,|\, Ug \rangle = \langle f \,|\, g \rangle \qquad \forall f,g \in \mathcal{C}[L]. \tag{168}$$

This definition is equivalent to the *unitarity condition*

$$\Leftrightarrow \quad U^{-1} = U^+. \tag{169}$$

To complete the list of ingredients for a quantum mechanical theory, we have to define a second class of operators that represent observables. To be physically interpretable, observables need to be *self-adjoint*

$$O : \mathcal{C}[L] \to \mathcal{C}[L] \tag{170}$$

$$\langle f \,|\, Og \rangle = \langle Of \,|\, g \rangle \qquad \forall\, f,g \in \mathcal{C}[L]. \tag{171}$$

They have only real eigenvalues (possible measurement results) and their eigenfunctions form a basis of the corresponding Hilbert space. In a finite setting, this is equivalent to

O, being *symmetric*[80]

$$O^+ = O. \tag{172}$$

6.2 Accessing Real Space by Means of Translations

To access our just set "discrete world", we first want to introduce its most important symmetry transformations: translations (subsection 6.2.1). The next subsection (6.2.2) is devoted to its generator, the momentum operator and the related discrete from of a derivative operator. In subsection 6.2.3, we define also the position operator and show how the these discrete operators act on certain test functions. With the position operator we can analyze the fundamental commutation relations in subsection 6.2.4. Finally in subsection 6.2.5, we compare these results to finite-difference representations by means of test functions. The comparison by means of our Hamiltonian model is discussed in section 7.1.

6.2.1 Translations as a Group

In this subsection, we want to introduce the translation group of our discrete setting. But to represent any operator in our discrete Hilbert space, we need to fix the boundary conditions. To apply group theoretical methods, the only possible choice are periodic boundaries so that the closure postulate holds. A translation $\mathcal{T}$ is described by a connection vector $\vec{z} = (z_1, z_2, z_3) \in L$[81]

$$\begin{aligned} &\mathcal{T}_{\vec{z}} : \mathcal{C}[L] \to \mathcal{C}[L] \\ &(\mathcal{T}_{\vec{z}} f)_{\vec{x}} = f_{\vec{x}+\vec{z} \mod N} \end{aligned} \tag{173}$$

From this definition, we are able to derive a matrix representation of the operator by using group theoretical methods. In order to do that, we have to prove that the set of all translations $T = \{\mathcal{T}_{\vec{z}} \,|\, \vec{z} \in L\}$ together with multiplication form an (Abelian) group:

1. $\mathcal{T}_{\vec{x}}, \mathcal{T}_{\vec{y}} \in T \Rightarrow \mathcal{T}_{\vec{x}} * \mathcal{T}_{\vec{y}} = \mathcal{T}_{\vec{x}+\vec{y}} \in T$
2. $\mathcal{T}_{\vec{x}} * (\mathcal{T}_{\vec{y}} * \mathcal{T}_{\vec{y}}) = (\mathcal{T}_{\vec{x}} * \mathcal{T}_{\vec{y}}) * \mathcal{T}_{\vec{y}}$
3. $\exists E = \mathcal{T}_{\vec{0}}$ with $\mathcal{T}_{\vec{x}} * E = E * \mathcal{T}_{\vec{x}} = \mathcal{T}_{\vec{x}} \quad \forall\, \mathcal{T}_{\vec{x}} \in T$

[80] In the continuous Hilbert space, self-adjointness is more complicated. For a well-defined theory, we have to handle the infiniteness of the Hilbert space. An operator on the whole $L^2[K]$ has an infinite domain. Therefore, in the continuum theory, symmetry is not sufficient for self-adjointness, because there are operators that change their domain after transposing. Nevertheless, for the Hilbert space over $L[K]$ for any subset of $K \in \mathbb{R}^3$, it was proven that any representation of the Poincaré group is self-adjoint.

[81] The Wigner convention would result in a minus sign in this definition: $\mathcal{T}^{Wigner}_{\vec{z}} f_{\vec{x}} \equiv f_{\vec{x}-\vec{z}}$.

4. $\forall \mathcal{T}_{\vec{x}} \in T \quad \exists \mathcal{T}_{\vec{x}}^{-1} = \mathcal{T}_{-\vec{x}}$ with $\mathcal{T}_{\vec{x}} * \mathcal{T}_{-\vec{x}} = E$

This is very easy to validate for (173) and we do not explicitly show it here. We now try to find the *unitary matrix representation* that $\mathcal{T}$ should have

$$U^{\mathcal{T}_{\vec{z}}} : L \to L \tag{174}$$

$$U^{\mathcal{T}_{\vec{z}}} f(\vec{x}) = f(\vec{x} + \vec{z}) \tag{175}$$

$$\left(U^{\mathcal{T}_{\vec{z}}}\right)^{-1} = \left(U^{T_{\vec{z}}}\right)^{+}. \tag{176}$$

It turns out, that the unitary representations of translations are directly linked to *Fourier-transformations*. As in the continuous case we can find the reciprocal space $\tilde{L}$ by a Fourier-Transform $\mathcal{F}$:

$$\tilde{f} = \mathcal{F}(f) : \tilde{L} \to \mathbb{C} \tag{177}$$

$$\tilde{f}_{\vec{k}} = \sum_{\vec{x} \in L} e^{-\mathbf{i}\vec{k}\cdot\vec{x}} f_{\vec{x}} = \sum_{\vec{x} \in L} e^{-\mathbf{i}\frac{2\pi}{N}(k_1 x_1 + k_2 x_2 + k_3 x_3)} f_{\vec{x}} \tag{178}$$

$$\text{with} \quad \vec{k} = \frac{2\pi}{N}(k_1, k_2, k_3) \quad k_l \in \{1, 2, \ldots, N\}/\Delta \quad l = 1, 2, 3 \tag{179}$$

and its back transformation $\mathcal{F}^{-1}$

$$\mathcal{F}^{-1}(\tilde{f}) : L \to \mathbb{C} \tag{180}$$

$$f_{\vec{x}} = \frac{1}{N^3} \sum_{\vec{k} \in L} e^{\mathbf{i}\vec{k}\cdot\vec{x}} \tilde{f}_{\vec{k}}. \tag{181}$$

We can easily deduce its matrix representation, when we combine the three spatial indices into one

$$\begin{pmatrix} f_{k_1} \\ f_{k_2} \\ \vdots \\ f_{k_{3N}} \end{pmatrix} = \begin{pmatrix} e^{\mathbf{i}k_1 \cdot x_1} & e^{\mathbf{i}k_1 \cdot x_2} & \ldots & e^{\mathbf{i}k_1 \cdot x_{3N}} \\ e^{\mathbf{i}k_2 \cdot x_1} & e^{\mathbf{i}k_2 \cdot x_2} & \ldots & e^{\mathbf{i}k_2 \cdot x_{3N}} \\ \vdots & \vdots & \ddots & \vdots \\ e^{\mathbf{i}k_{3N} \cdot x_1} & e^{\mathbf{i}k_{3N} \cdot x_2} & \ldots & e^{\mathbf{i}k_{3N} \cdot x_{3N}} \end{pmatrix} \cdot \begin{pmatrix} f_{x_1} \\ f_{x_2} \\ \vdots \\ f_{x_{3N}} \end{pmatrix}. \tag{182}$$

Both spaces are equivalent, but their units and the distance between two neighboring points differ. The latter is given for any coordinate x_i by the spacing Δ[82]

$$x_{i,min} = \Delta \qquad \forall i \tag{183}$$

[82] To keep things simple, we defined a uniform grid in the beginning of this chapter.

for the real space, and

$$k_{i,min} = \frac{2\pi}{N\Delta} \qquad \forall i \tag{184}$$

for the reciprocal (k)-space $k_{i,min}$.

The irreducible representation of discrete translations can be found for example in Wagner [1998]. It is the multiplication by a complex number with absolute value equal to one in the reciprocal space:

$$\begin{aligned}
(\mathcal{T}_{\vec{z}} f)_{\vec{x}} &= \mathcal{F}^{-1} e^{\mathbf{i}\vec{k}\cdot\vec{z}} \mathcal{F}(f) \\
&= \mathcal{F}^{-1} \left(e^{\mathbf{i}\vec{k}\cdot\vec{z}} \sum_{\vec{y}\in L} e^{-\mathbf{i}\vec{k}\cdot\vec{y}} f_{\vec{y}} \right) \\
&= \frac{1}{N^3} \sum_{\vec{k}\in\tilde{L}} e^{\mathbf{i}\vec{k}\cdot\vec{x}} e^{\mathbf{i}\vec{k}\cdot\vec{z}} \sum_{\vec{y}\in L} e^{-\mathbf{i}\vec{k}\cdot\vec{y}} f_{\vec{y}} \\
&= \frac{1}{N^3} \sum_{\vec{k}\in\tilde{L}} e^{\mathbf{i}\vec{k}\cdot(\vec{x}+\vec{z})} \sum_{\vec{y}\in L} e^{-\mathbf{i}\vec{k}\cdot\vec{y}} f_{\vec{y}} \\
&= f_{\vec{x}+\vec{z}}
\end{aligned} \tag{185}$$

The same identity exists in continuous theory

$$f(x+y) = \frac{1}{2\pi} \int \mathrm{d}k\, e^{\mathbf{i}k(x+y)} \int \mathrm{d}x' e^{-\mathbf{i}kx'} f(x'). \tag{186}$$

The construction of the unitary representation of elements of $\mathcal{T}$ shows us already how to change to its *eigen-representation*. We first formally decompose the operator

$$(\mathcal{T}_{\vec{z}} f)_{\vec{x}} = \sum_{\vec{y}\in L} \sum_{i=1}^{3N} a_i \langle \vec{x} \,|\, \Phi_i \rangle \langle \Phi_i \,|\, \vec{y} \rangle \langle \vec{y} \,|\, f \rangle \tag{187}$$

$$\text{with } (\mathcal{T}_{\vec{z}} f)_{\vec{x}} \,|\Phi_i\rangle = a_i \,|\Phi_i\rangle \,. \tag{188}$$

$$\tag{189}$$

Now we compare it to the unitary representation

$$(\mathcal{T}_{\vec{z}} f)_{\vec{x}} = \frac{1}{N^3} \sum_{\vec{k}\in\tilde{L}} e^{\mathbf{i}\vec{k}\cdot\vec{x}} e^{\mathbf{i}\vec{k}\cdot\vec{z}} \sum_{\vec{y}\in L} e^{-\mathbf{i}\vec{k}\cdot\vec{y}} f_{\vec{y}} \tag{190}$$

$$f_{\vec{y}} \to \langle \vec{y} \,|\, f \rangle \tag{191}$$

$$e^{-\mathbf{i}\vec{k}\cdot\vec{y}} \to \langle \Phi_i \,|\, \vec{y} \rangle \tag{192}$$

$$a_i \to e^{\mathbf{i}\vec{k}\cdot\vec{z}} \tag{193}$$

$$e^{\mathbf{i}\vec{k}\cdot\vec{x}} \to \langle \vec{x} \,|\, \Phi_i \rangle \,. \tag{194}$$

We see that the Fourier-transformation is actually the transformation from position coordinates to the eigenfunctions of translations which are reciprocal coordinates. The eigenvalues are just complex exponentials. We see here that translation operators are not self-adjoint. We can also conclude that all operators and states that are diagonal in Fourier-space are *translational invariant*.

6.2.2 Momentum Operator and Derivatives

It is important to emphasize that $\mathcal{T}$ is unitary and *not* self-adjoint, hence it does not correspond to any observable. But we can now construct a self-adjoint operator that is diagonal in Fourier-space, which means that the vectors $\Phi_{\vec{k}}$, that were introduced in the last subsection, are its eigenvectors. This simplest possible self-adjoint operator that shares its eigenfunctions with translations would be

$$\begin{aligned}\mathcal{P}f &= \sum_{\vec{k}\in\tilde{L}} \vec{k}\,\big|\Phi_{\vec{k}}\big\rangle\big\langle\Phi_{\vec{k}}\,\big|\,f\big\rangle \\ &= \frac{1}{N^3}\sum_{i=1}^{3N} e^{\mathbf{i}k_i\cdot\vec{x}}k_i \sum_{\vec{y}\in L} e^{-\mathbf{i}\vec{k}\cdot\vec{y}}f_{\vec{y}}. \end{aligned} \tag{195}$$

This definition seams to be reasonable, as it has the right continuum limit $\mathcal{P}_{cont} = -\mathbf{i}\partial_x$

$$\begin{aligned}\mathcal{P}_{cont}f(x) &= -\mathbf{i}\partial_x f(x) \\ &= -\mathbf{i}\partial_x \frac{1}{(2\pi)^3}\int \mathrm{d}k\, e^{\mathbf{i}kx}\int \mathrm{d}y\, e^{-\mathbf{i}ky}f(y) \\ &= -\mathbf{i}\frac{1}{(2\pi)^3}\int\int \mathrm{d}y\mathrm{d}k\,\partial_x e^{\mathbf{i}k(x-y)}f(y) \\ &= -\mathbf{i}\frac{1}{(2\pi)^3}\int\int \mathrm{d}y\mathrm{d}k\,\mathbf{i}k e^{\mathbf{i}k(x-y)}f(y). \end{aligned} \tag{196}$$

We want to remark that this approach is computationally fast, when we implement it by means of the fast Fourier transform algorithm, as already Feit et al. [1982] argued.

Finally, let us also define the *nth derivative operator*

$$(\partial_i)^n f = \frac{1}{n!}\mathcal{F}^{-1}((\mathbf{i}k_i)^n(\mathcal{F}f)_{\vec{k}}), \tag{197}$$

$$\partial_i f(\vec{y}) = \frac{1}{N^3}\sum_{\vec{k}\in L} e^{\mathbf{i}\frac{2\pi}{N}(k_1y_1+k_2y_2+k_3y_3)}\mathbf{i}k_i \sum_{\vec{x}\in L} e^{-\mathbf{i}\frac{2\pi}{N}(k_1x_1+k_2x_2+k_3x_3)}f_{\vec{x}} \tag{198}$$

$$= \frac{1}{N^3}\sum_{\vec{k}\in L} e^{\mathbf{i}\vec{k}\cdot\vec{y}}\mathbf{i}k_i \sum_{\vec{x}\in L} e^{-\mathbf{i}\vec{k}\cdot\vec{x}}f_{\vec{x}} \tag{199}$$

$$= \frac{1}{N^3}\sum_{\vec{k},\vec{x}} \mathbf{i}k_i e^{\mathbf{i}\vec{k}\cdot(\vec{y}-\vec{x})}f_{\vec{x}}. \tag{200}$$

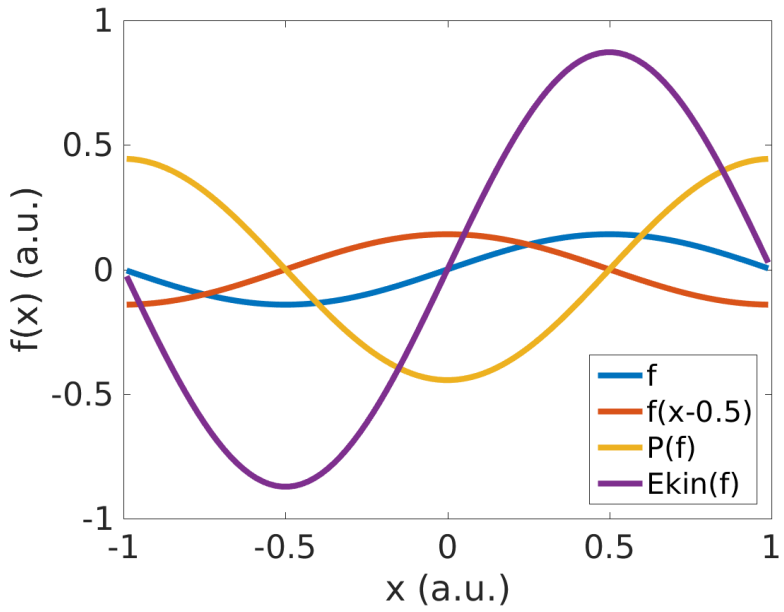

FIG. 13: We show the test function $f : L \to L, f(x) = \sin(x)$ and the action of the operators of the last subsection on it: the translation, momentum and kinetic energy operator. The all act, as expected from the continuum limit.

Note that every operator for odd derivatives has purely imaginary eigenvalues and consequently is not self-adjoint. Thats why we need to add the **i** in the definition of the momentum. As special case, we define the non-relativistic kinetic energy operator $\mathcal{K}$ analogously to $\mathcal{P}$ as $\mathcal{K} = -\mathcal{P}^2/2$

$$\mathcal{K}f : \mathcal{C}[L] \to \mathcal{C}[L] \tag{201}$$

$$\mathcal{K}f = \frac{1}{2N^3} \sum_{i=1}^{3N} e^{\mathbf{i}k_i \cdot \vec{x}} (k_i)^2 \sum_{\vec{y} \in L} e^{-\mathbf{i}\vec{k}\cdot\vec{y}} f_{\vec{y}}. \tag{202}$$

6.2.3 The Action of Translations

In this subsection, we want to visualize the new definitions in one dimension. For that, we show two examples for the action of the developed operators on test functions. Figure 13 shows the function $f : L \to \mathbb{R}$, $f(x) = \sin(x)$, that is one eigenmode of the "periodic resonator." We see, that all our defined operators act exactly as we expect: Translations translate the coordinates of the function f, the momentum operator P gives the negative derivative of f and the kinetic energy operator applied to f is proportional to the function itself. We also verified that the amplitudes correspond to the continuous limit operators. The second example is shown in figure 14. The text function here is $f : L \to \mathbb{R}$, $f(x) = x$, that was translated by means of the developed formalism. Here we see well how important the domain of the function is: we defined a certain function $f : L \to \mathbb{R}$ that has in fact

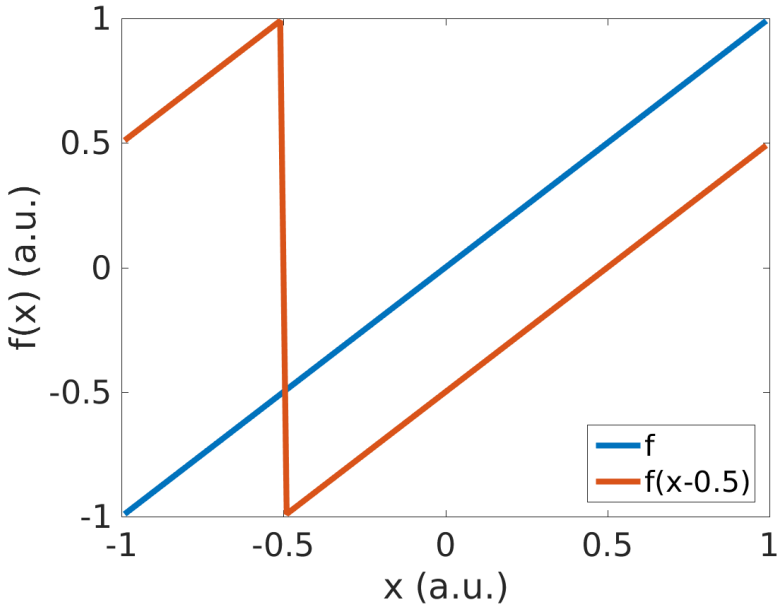

FIG. 14: The test function $f : L \to L, f(x) = x$ and the action of the $z = 0.5$ translation operator (185) on f is shown. As expected, we see the coordinate change in x.

the same rule like the identity on $\mathbb{R} : f : \mathbb{R} \to \mathbb{R}, f(x) = x$. But on L with periodic boundary conditions, it is a sawtooth function with very steep jump. Consequently, its continuous limit can never be part of the domain of any differential operators. For pure translations there is no difference, but we see in subsection 6.2.5, how the jump visualizes the differences to the finite-differences method.

6.2.4 Discrete Commutation Relations

In this subsection, we first introduce and discuss the position operator of our discrete lattice. Then we use this expression to define the fundamental commutation relations.

To demonstrate the concepts that were developed so far, let us have a look at the position operator $\hat{\vec{x}}$[83] that measures the position of an object in our space. As we defined the space in position space we already used its *eigenrepresentation*

$$\hat{\vec{x}} : L \to L \tag{203}$$

$$\hat{\vec{x}} f(\vec{y}) = (\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_{3N}) f(\vec{y}) \tag{204}$$

$$\hat{\vec{x}} f(\vec{y}) = \sum_{\vec{y} \in L} \sum_{i=1}^{3N} a_i \langle \vec{z} \,|\, x_i \rangle \langle x_i \,|\, \vec{y} \rangle \langle \vec{y} \,|\, f \rangle \tag{205}$$

[83] We denoted the vector operator $\hat{\vec{x}}$ with a hat to distinguish it from the coordinate $\vec{x}$. Other operators are *not* denoted by a hat like in other chapters.

$$= \sum_{i=1}^{3N} a_i \langle x_i \,|\, f \rangle \,. \tag{206}$$

The eigenvalues a_i are of course translational invariant, but within a certain representation we need to specify one origin. Here, we need to distinguish between two situations. Either there is a distinguished origin or not. Such origin could be defined by the experimental setting, like for example the monopole of a charge distribution that is the origin for the dipole operator. We want to show the difference in a small Gedankenexperiment. Let us assume that we want to make a measurement of the position of a test function (in only 1 dimension):

$$\langle \hat{x} \rangle_f = \sum_{i=1}^{N} \langle f \,|\, x_i \rangle \, a_i \, \langle x_i \,|\, f \rangle \tag{207}$$

$$= a_1 |f(x_1)|^2 + a_2 |f(x_2)|^2 + \cdots + a_N |f(x_N)|^2 \tag{208}$$

$$\overset{\text{standard}}{=} 0|f(x_1)|^2 + 1|f(x_2)|^2 + \cdots + (N-1)|f(x_N)|^2. \tag{209}$$

If we would have a very peaked function with only one entry, like

$$f_p(x_1) = 1, \; f_p(x_i) = 0 \qquad \text{for } i = 2, 3, \ldots N, \tag{210}$$

our standard definition would result as we want in $\langle \vec{x} \rangle_{f_p} = 0 = x_1$. But what happens if we translate the coordinate system by an arbitrary distance?

$$\langle \mathcal{T}_z x \rangle_f = \sum_{i=1}^{N} \langle f \,|\, \mathcal{T}_z \,|\, x_i \rangle \, \mathcal{T}_z a_i \, \langle x_i \,|\, \mathcal{T}_z \,|\, f \rangle \tag{211}$$

$$= \sum_{i=1}^{N} \langle f \,|\, x_i + z \rangle \, (\mathcal{T}_z a_i) \, \langle x_i + z \,|\, f \rangle \tag{212}$$

$$= (\mathcal{T}_z a_1)|f(x_1 + z)|^2 + \cdots + (\mathcal{T}_z a_N)|f(x_N + z)|^2 \tag{213}$$

$$\tag{214}$$

For vectors, the translation is well defined but we do not know *how $\mathcal{T}$ acts on the eigenvalues of an operator*. We summarize the two possibilities:

1. $T_z a_i = a_i + z \rightarrow \langle \mathcal{T}_z \hat{x} \rangle_f = \langle \hat{x} \rangle_f$, so the origin is distinguished and e.g. a dipole moment would not change under the actions of a translation or

2. $T_z a_i = a_i \rightarrow \langle \mathcal{T}_z \hat{x} \rangle_f = \sum_{i=1}^{N} \langle f \,|\, x_i + z \rangle \, a_i \, \langle x_i + z \,|\, f \rangle$, so it does not act on the eigenvalues which corresponds to a normal position measurement

Consider for example a translation by 2

$$\begin{aligned}\langle \mathcal{T}_{z=2}\hat{x}\rangle_{f_p} &\overset{1.}{=} 2|f_p(x_3)|^2 + 3|f_p(x_4)|^2 + \cdots + 0|f_p(x_1)|^2 + 1|f_p(x_2)|^2 \\ &= 0|f(x_1)|^2 + 1|f(x_2)|^2 + \cdots + (N-1)|f(x_N)|^2 \\ &= 0 \\ &\overset{2.}{=} 0|f_p(x_3)|^2 + 1|f_p(x_4)|^2 + \cdots + (N-1)|f_p(x_2)|^2 \\ &= N-2\end{aligned}$$

Of course we could also say that the dipole operator is invariant under translations but the position operator is not.

Let us now use this definition to analyze the discrete fundamental commutator between position $\hat{x}$ and momentum $\hat{p}$. Commutation relations are essential in quantum physics and in a way they set a limit to discretized theories. This is because of the finiteness of the theory. It can be proven [v. Neumann, 1931], that the fundamental commutator between position $\hat{x}$ and momentum $\hat{p}$

$$[\hat{x}, \hat{p}] = 1 \tag{215}$$

can only be fulfilled if one of two operators is unbounded.

Instead, the commutation relation in the discretized theory has a commutation rest $R(N)$

$$\begin{aligned}\hat{x}_i\hat{p}_i f(\vec{x}) &= \mathbf{i}x_i \frac{1}{N^3}\sum_{\vec{k},\vec{y}} \mathbf{i}k_i e^{\mathbf{i}\vec{k}\cdot(\vec{x}-\vec{y})} f_{\vec{y}} \\ \hat{p}_i\hat{x}_i f(\vec{x}) &= \mathbf{i}\nabla(x_i f_{\vec{x}}) = \mathbf{i}f_{\vec{x}}\nabla x_i + \mathbf{i}x_i\nabla f_{\vec{x}} \\ &= \mathbf{i}f_{\vec{x}}\frac{1}{N^3}\sum_{k_i,y_i} \mathbf{i}k_i e^{\mathbf{i}k_i(x_i-y_i)} y_i + \mathbf{i}x_i \frac{1}{N^3}\sum_{\vec{k},\vec{y}} \mathbf{i}k_i e^{\mathbf{i}\vec{k}\cdot(\vec{x}-\vec{y})} f_{\vec{y}} \\ \Rightarrow [\hat{x}_i, \hat{p}_i] f(\vec{x}) &= \mathbf{i}f_{\vec{x}}\frac{1}{N^3}\sum_{k_i,y_i} \mathbf{i}k_i e^{\mathbf{i}k_i(x_i-y_i)} y_i \\ &= \mathbf{i}R(N) f_{\vec{x}}.\end{aligned} \tag{216}$$

The commutation rest $R(N)$ is for finite grid size N not the $\mathbb{1}$ matrix, but

$$R(N) \equiv \frac{1}{N^3}\sum_{k_i,y_i} \mathbf{i}k_i e^{\mathbf{i}k_i(x_i-y_i)} y_i \neq \mathbb{1}. \tag{217}$$

Instead in the continuous limit, we would have:

$$[\hat{x}, \hat{p}] f(x) = \mathbf{i}f(x)\frac{1}{(2\pi)^3}\int\int \mathrm{d}y\mathrm{d}k\, \mathbf{i}k e^{\mathbf{i}k(x-y)} y \tag{218}$$

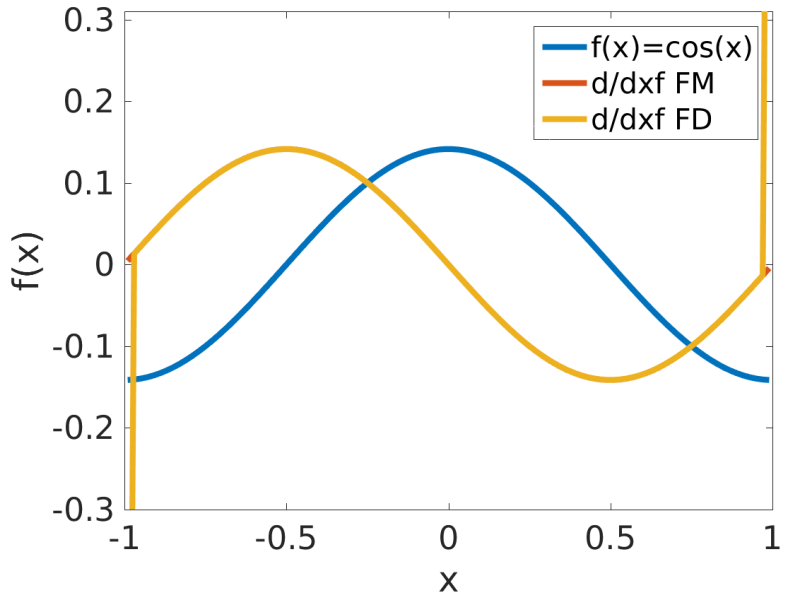

FIG. 15: We that both, the FD and FM method behave neraly identically. The deviation is due to Dirichlet boundary conditions being imposed on the FD operator.

$$= \mathbf{i} f(x) \frac{1}{(2\pi)^3} \int \int \mathrm{d}y \mathrm{d}k \, \partial_x e^{\mathbf{i}k(x-y)} y \tag{219}$$

$$= \mathbf{i} f(x) \partial_x \frac{1}{(2\pi)^3} \int \mathrm{d}k e^{\mathbf{i}kx} \int \mathrm{d}y \, e^{-\mathbf{i}ky} y \tag{220}$$

$$= \mathbf{i} f(x) \partial_x \frac{1}{(2\pi)^3} \int \mathrm{d}k e^{\mathbf{i}kx} (\mathcal{F}\,\mathrm{id})_k \tag{221}$$

$$= \mathbf{i} f(x) \partial_x x \tag{222}$$

$$= \mathbf{i} f(x), \tag{223}$$

where we used the inverse of the proof (196). In the continuous limit, the commutation relations are fulfilled.

In equation (140), we saw this rest already in the respective form for the Bosonic commutators.

6.2.5 Comparison to Finite Differences

Lastly, we want to compare both methods to discretize operators, finite-differences (FD) and the just presented Fourier-method (FM).

We start again by means of a mode function of the domain: $f : L \to \mathbb{R}$, $f(x) = \cos(x)$. We see that both method are (nearly) identically. Only close to the domain boundary, the finite-differences method exhibits a deviation. But this is simply because we have imposed Dirichlet boundary conditions. There is only one of the two terms of the central

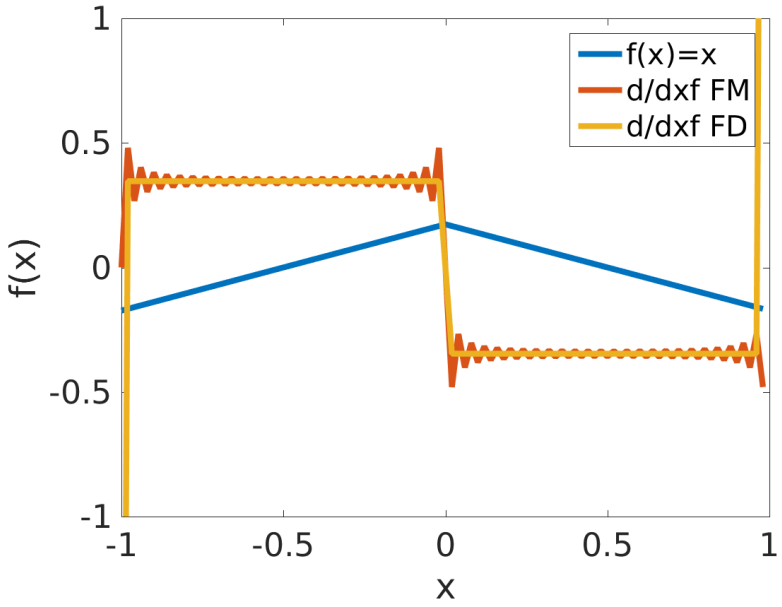

FIG. 16: Differences are best stressed by a function that would not be in the domain of any operator in the continuous case, a not differentiable ramp function. Here we see that FD (nearly) recovers the behavior of a derivative but FM „presses“ it into its domain.

differences method at the boundary. We checked that both methods agree with periodic boundary conditions up to the discretization error.

Now we want to demonstrate the differences between both methods. We apply the operators on a function, that is not part of the domain of the respective continuous limit: the ramp function $f(x) \propto -|x|$. In figure 16, we can see what this means. The FD operator (nearly) recovers the behavior of a derivative. But the FM derivative exhibits a “wiggle”-structure. These could be called the ghosts of the discontinuities from the continuous limit. In this sense, the FM operator “knows” about its continuum limit or more precisely, about the domain of it.

From these results we see that both methods obviously exhibit differences and that their comparison is worth analyzing further: this is done in chapter 7.

6.3 Other Symmetry Operators

Beside translations, a general cubic grid exhibits some more symmetries. These are the 48 different symmetry transformations, consisting of all possible rotations and reflections [Wagner, 1998]. In theory it is thus possible to construct something like the angular momentum operator for such a grid, what we spare here. Anyway, such an operator may define certain rotations, but they do not change, when the number of grid points is varied. Hence, the continuous limit is approached non-continuously.

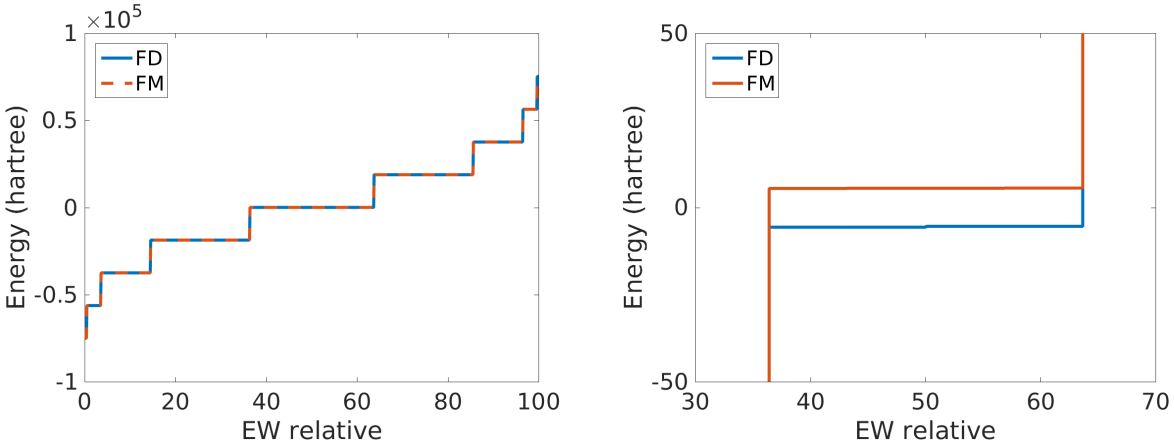

FIG. 17: Comparison of the eigenvalues of the Hamiltonian for FD and FM method. We see that they look exactly the same on large scales (left), but zooming closer, we see deviations (right).

7 Numerical Results of the Fourier Method

In this last chapter, we want to present the first results, that we obtained with the Fourier method. In the first section (7.1) we present the energy spectra of the Fourier-Hamiltonian in comparison with the finite-differences method. There we see that both methods have indeed a different behavior. We can proof that is due to a different spacing dependency.

In the second section (7.2), we try to analyze the commutator between the Hamiltonian and the momentum for the full interacting theory. We show that it does not vanish, because of the commutation rest between Boson operators.

7.1 Comparison to Finites-Differences

In this section, we finally compare the finite-differences (FD) and the Fourier methods (FM). To properly do that, we impose periodic boundary conditions on the finite-differences Hamiltonian.[84]

In figure 17, we see the comparison between the energy spectrum of the FM and FD method. On big scales, their lines entirely overlap in the plot, but closely around the energy plateaus, there are deviations. Let us analyze this more precisely: The difference between both methods is mainly due to a different dependence on Δ_x. Therefore, let us briefly recapitulate the terms of the Hamiltonian and its dependence on Δ_x. The Hamiltonian consists of five terms[85]

$$H = H_{mass} + H_{kin} + H_{int} + H_{mag} + H_{elec}, \tag{224}$$

[84] We mentioned the deviations in 4.2.
[85] We dropped the hat symbol to denote operators in this chapter for simplicity.

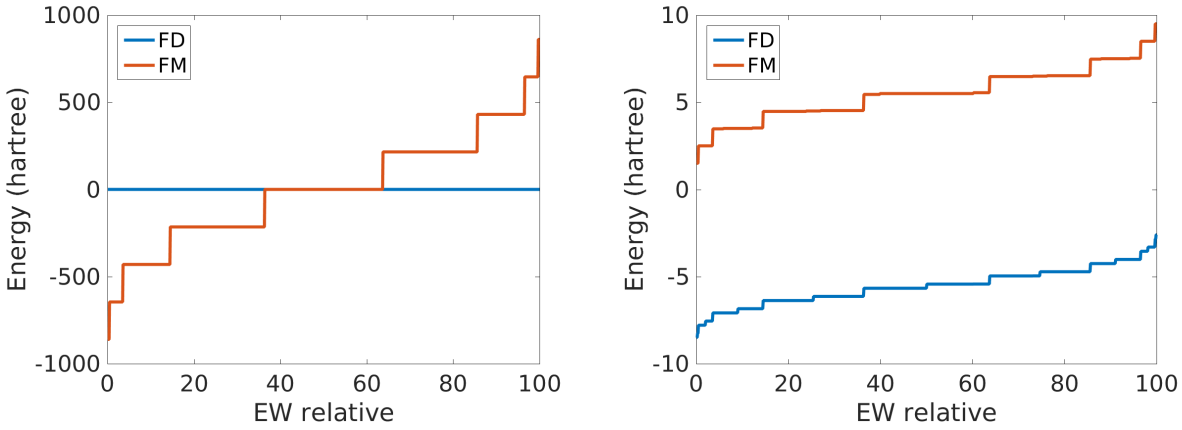

FIG. 18: We see the different contributions of the spectra of the FD and FM method. The momentum contribution in FM (left) is on a medium energy scale up to ±1000 Hartree but the FD momentum term vanishes. Likewise, for the sum of interaction and electromagnetic part (that are on the same scale), we can observe deviations.

that are all functions of Δ_x with very different dependencies:

$$H_{mass} = mc^2 \int_{\mathbb{R}^3} \mathrm{d}^3 r\, \psi^+ \beta \psi \qquad \propto \frac{1}{\Delta_x} \tag{225}$$

$$H_{kin} = -\mathbf{i}\hbar c \int_{\mathbb{R}^3} \mathrm{d}^3 r\, \psi^+ \vec{\alpha} \cdot \nabla\, \psi \qquad \propto \frac{1}{\Delta_x^2} \tag{226}$$

$$H_{int} = -e \int_{\mathbb{R}^3} \mathrm{d}^3 r\, \psi^+ \vec{\alpha} \cdot \vec{A} \psi \qquad \propto \frac{1}{\sqrt{\Delta_x^3}} \tag{227}$$

$$H_{mag} = \frac{\epsilon_0}{2} \int_{\mathbb{R}^3} \mathrm{d}^3 r\, \left(\nabla \times \vec{A}\right)^2 \qquad \propto \frac{1}{\Delta_x^3} \tag{228}$$

$$H_{elec} = \frac{\epsilon_0}{2} \int_{\mathbb{R}^3} \mathrm{d}^3 r\, \left(c\vec{E}\right)^2 \qquad \propto \frac{1}{\Delta_x}. \tag{229}$$

We see, that H_{mass} and H_{elec} have to weakest dependency on Δ_x and hence they will be dominated by the others for small spacing.

For our standard choice $\Delta_x = 1$ (Bohr) instead, we already know from chapter 5, that the mass term is dominating over any other. Yet we can expect that this will change for small Δ_x. Figure 18 confirms this guess. We also see in the figure another feature of the finite-differences method with periodic boundary conditions: the momentum operator is zero, because all the contributions cancel out each other pairwise. This of course is a very inconvenient fact, especially when we compare it to the Fourier method, which shows high eigenvalues for the momentum operator.

Let us now analyze the derivations of the FD-Hamiltonian with respect to Δ_x. From our previous considerations we can guess that we will observe exchanges of the dominating energy contributions. We compare both spectra under variation of Δ_x in figure 19. Although the energy values approach each other for $\Delta_x = 1$, there are strong deviations for small Δ_x. These are due to the different growth of all the terms but the mass and the

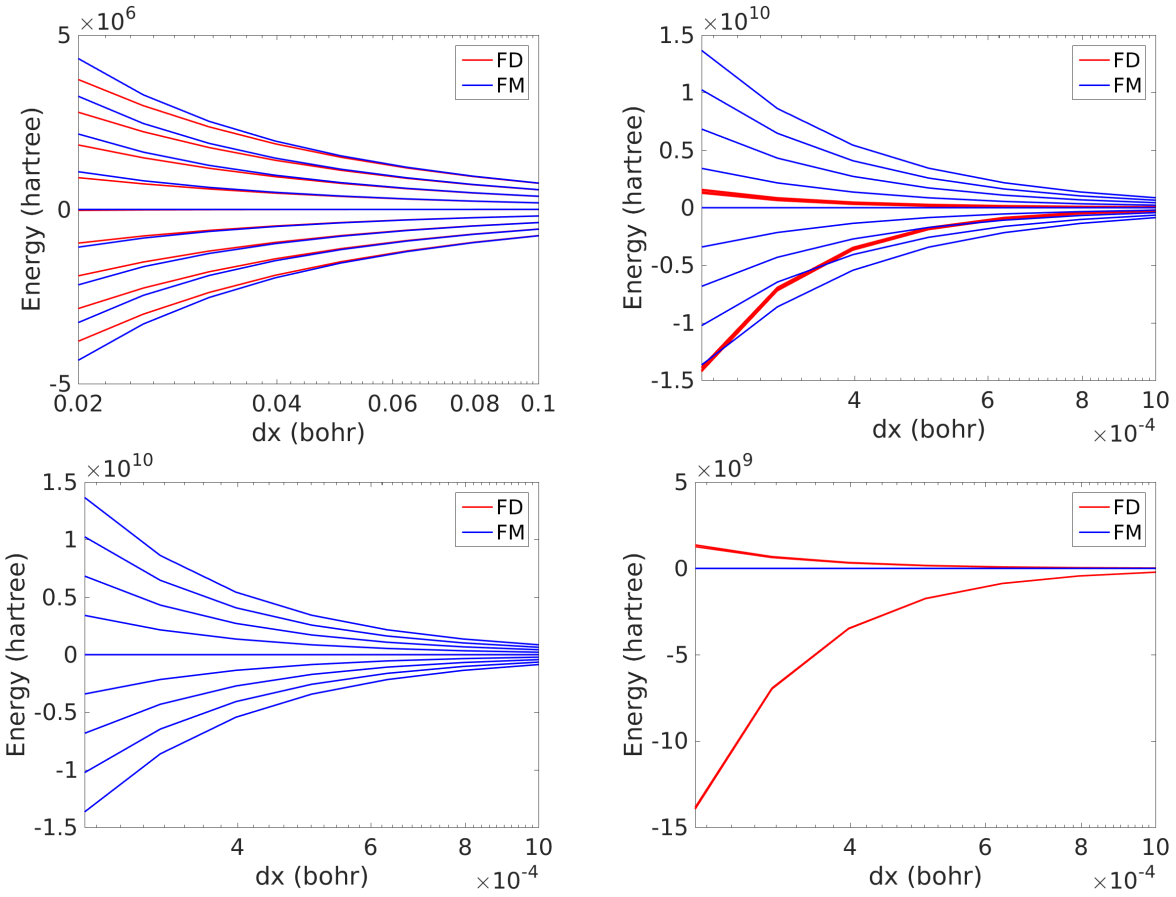

FIG. 19: The FD and FM method are compared under variation of the spacing Δ_x. For $\Delta_x \approx 0.1$, the respective energy values become nearly identically (up,left). But for smaller Δ_x, both methods deviate strongly (up,right). This is due to the growth of the momentum term (down,left), the interaction and the electric term (down,right).

electric term H_{mass}, H_{elec}.

We also repeated the other parameter variations, but we did not find comparable, qualitative differences between the Fourier and finite-differences method.

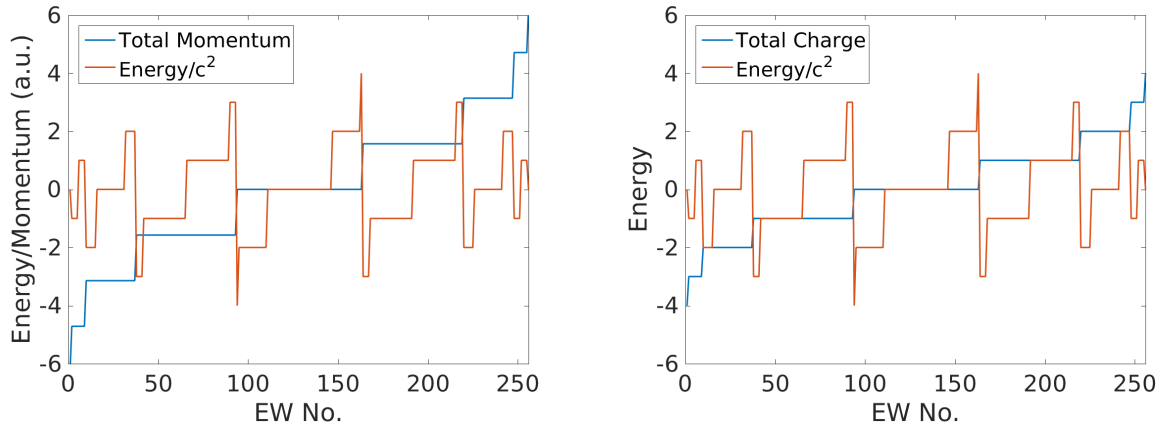

FIG. 20: The eigenvalue spectrum of the Dirac Hamiltonian, reordered by two different symmetry operators. On the left, we block-diagonalized the Hamiltonian by means of the total momentum operator and on the right, we show its reordered spectrum according to the charge operator. The energy spectrum is exactly equivalent.

7.2 Remarks on Symmetries in Full QED

In this last section, we want analyze the translation symmetry of the Hamiltonian with the aid of the Fourier method.

We want to start again with the bare Dirac Hamiltonian like in section 5.4. For the sake of completeness, we show in figure 20 the eigenvalues of the Hamiltonian in the Fourier method that was block-diagonalized with the aid of the momentum operator. Due to numerical problems, we could not perform this operation for the finite-differences case. It is compared to the corresponding figure of the block-diagonalization by means of the charge operator in the Fourier method.[86] Interestingly, the energy eigenvalues are exactly equivalent.

Having confirmed the translational invariance of the free theory, the logical next step is to analyze the [H,P]-commutator in the full interacting theory. The P operator is then generalized to

$$\vec{P} = \int \mathrm{d}^3 r \psi^+ \left(-\mathbf{i}\hbar\nabla - e\vec{A} \right) \psi, \tag{60}$$

so it consists of the canonical part

$$\vec{P}_{can} = -\mathbf{i}\hbar \int \mathrm{d}^3 r \psi^+ \nabla \psi, \tag{230}$$

[86] It is equivalent to figure 12 of subsection 5.3.1, where the same is already shown for finite-differences. As the charge operator does not depend on the discretization method, this equivalence could be expected.

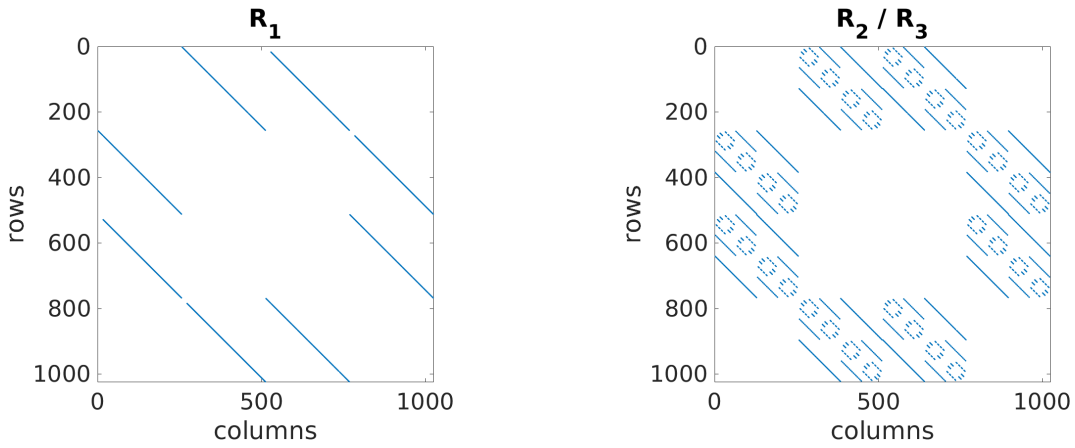

FIG. 21: We see the three different parts of commutator between H and P): One of them is due to the fundamental Bosonic commutation rest (left, R_1). The second and the third contribution have the same sparsity pattern (right, R_2, R_3). See text for further explanations.

and a part, with Bosonic contribution

$$\vec{P}_{bos} = -e \int \mathrm{d}^3 r \psi^+ \vec{A} \psi. \tag{231}$$

As expected, the commutator between the Hamiltonian and the canonical momentum does not vanish. In figure 21 instead, we show the commutation rest. It has three parts: first, the contribution from the Bosonic parts of the Hamiltonian $H_{bos} = H_{int} + H_{electric} + H_{magnetic}$ and the momentum

$$R_1 = [H_{bos}, \vec{P}_{bos}], \tag{232}$$

second, the contribution from H_{int} and the canonical momentum

$$R_2 = [H_{int}, \vec{P}_{can}], \tag{233}$$

and last, another contribution from the Bosonic momentum, but this time with the kinetic part of H

$$R_3 = [H_{in}, \vec{P}_{bos}]. \tag{234}$$

The first part R_1 is due to the truncation error of the Bosonic commutators that was discussed in subsection 4.3.1. If we want to find the block-diagonalized form of the full interacting Hamiltonian, we have to find a way to eliminate the truncation error. This will be topic of future research.

For the latter two parts R_2, R_3, this is different. Interestingly, both have exactly the same sparsity structure. And not only that, the difference between both matrices is only a real

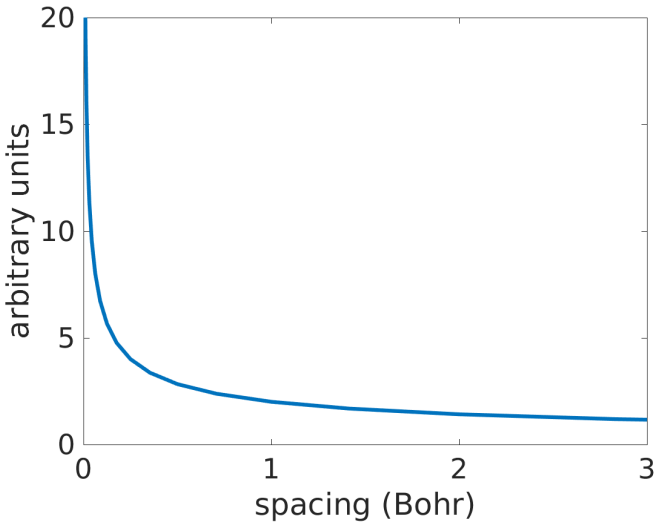

FIG. 22: We see the factor between the two commutation rests

factor

$$f = R_{2,ij}/R_{3,ij} \qquad \forall i, j. \tag{235}$$

By manually multiplying the Bosonic part of the momentum operator P_{bos} with this factor

$$P_{bos}^{fix} = f \cdot P_{bos}, \tag{236}$$

both contributions cancel out each other

$$R_3^{fix} = [H_{in}, P_{bos}^{fix}] = -R_2. \tag{237}$$

Only the Bosonic rest R_1 remains.

Interestingly, we found out that the factor varies with the spacing Δ_x (see figure 22). This is again a hint for a renormalization effect, that can be the object of further research.

8 Conclusion

The content of this thesis is rather diverse. We presented a technique to discretize quantum field theories. This was achieved by means of a mode expansion and the interpretation of the resulting terms in the sense of second quantization. But this is not enough to discretize differential equations. We have to decide how differential operators act on the discrete fields. Especially because it is computationally very efficient, a very common way in numerical analysis to handle this is the *finite-differences* method. But we also developed a different approach, which is based on the group theoretical interpretation of physical theories. By means of representation theory, the differential operators in a field theory are representations of certain generators of the group. In the second approach, we treated the differential operators as representations of the (discrete) symmetry group of the discretized space. This is mathematically equivalent to solving differential equations with the aid of Fourier transformations. (But in terms of physics, this gives us a different interpretation and connection to symmetries.)

We applied these methods on a Hamiltonian-based theory of quantum electrodynamics. We derived two different discrete expressions of the Hamiltonian and implemented them in a code. One of the main advantages of our approach is that it allows for analyzing the complete (discrete) Fock space of the theory. The price for that is like usual in interacting quantum theories, that we are restricted to very small model systems.

Nevertheless, the developed methods form a good framework to analyze the fundamental problems of QED like renormalization, or the negative energy solutions of the Hamiltonian. We see that traces of all of them are still present in our small system. Even our very small model system allows for visualizing certain limit cases. This is good to verify the theory, so we are able to see that the non-relativistic, the strong-coupling, and the heavy-Fermion limit is reasonable. Moreover, we are able to visualize the transition between the general theory and its limits. We can observe which eigenvalues degenerate to one energy manifold and where. Or if and where there are line-crossings. In future work, we want to compare this to certain analytically derived limit cases like the Pauli equation for the non-relativistic limit, so that we can identify where and how the theories deviate. One could also include higher order terms, etc.

As we have access to the complete Fock space, we can study the role of symmetries in a remarkable way. We can track how a Hamiltonian in any basis is symmetrized due to any symmetry operator. This just corresponds to a block-diagonalization in our matrix picture. For example, we have illustrated that the total charge operator divides the QED-Hamiltonian in $L = 4N + 1$ blocks of different charge eigenvalues. But the framework is very general and we can redo this (theoretically) for any symmetry.

And finally, we can investigate the role of the discretization itself. We found that especially

the behavior under spacing variations depends strongly on the discretization method. Both our methods have a very different energy spectrum for strong confinement. This is connected to renormalization. To compare the energies for different Δ_x values, we need to properly renormalize the theory. The unequal behavior of the two methods is a hint for a difference in their renormalization procedures, especially because the differential operators, that "carry the difference" between both methods, have the same continuous limit.

We also directly see the commutation errors arising from the truncation of the Bosonic space. This was visible when we analyzed the commutation error between the Hamiltonian and the momentum for the full interacting theory. We were able to identify two reasons: one is spacing dependent and probably also linked to renormalization, and we were able to eliminate it by inserting an artificial factor. Yet another error remained from all the terms with Bosonic operators, and we could show that this is exactly due to the Bosonic truncation error. One of our future projects is to apply methods to also eliminate that error. Our framework should be perfectly suited to analyze such a procedure with all its implications.

In conclusion, we were able to develop a framework that is very promising for the investigation of discretization. As noted in the introduction, our work was guided by three research questions. The first and most general of our research question was "what is the influence of the discretization on the ingredients of a physical theory: equations of motion, spinor-wave fields and symmetries." From our results we can conclude that there is definitely an influence, but that it is very difficult to quantify its importance. Especially symmetries are broken in discretized settings, and the derivation of spinor algebras or covariant equations of motion as representations of something like a "discrete Minkowski space" are not possible in our point of view. Maybe there are generalizations of group theory possible that could allow for that, but we did not investigate this more deeply.

The second question was "whether it matters, *on which level* the discretization takes place." This questions is definitely not answered so far, but at least we can say that our analyzed limit cases look qualitatively reasonable. But quantitative and precise answers definitely need larger grids. The possibility of comparing QED with a limit case before and after the discretization is mentioned in the outlook.

The third and last question was "whether the discretization methods differ crucially." This turned out to be a very promising research topic for our model, because we indeed found a difference between our two discretization methods. The deeper reasons for this are still to be found and the results could be very important for theories that have to deal with any renormalization.

9 Outlook

As the development of our new approach is still at a very early stage, this outlook is probably an especially important part. We hope that the reader shares our opinion that the developed framework presents a big potential. A lot of the possible future applications were already mentioned in the respective chapters and we do not want to repeat all of them. Here, we focus on the most important part from our perspective, where some of them are already in process.

To complete our survey on symmetries is essential for lots of other things. We aim to maximally block-diagonalize the Hamiltonian with the aid of all possible symmetry operators. With this, we hope to find an effective algorithm that gives us any of these blocks *without* the necessity of building the whole Fock space. This is especially important to make studies on bigger domains feasible. We saw already that the truncation error of the fundamental Bosonic commutation relations is an important obstacle to such block-diagonalizations. A possible way to clear this could be a method called "discrete canonical commutation relations" [Hammel, 2004] or the use of finite Bosonic oscillators (e.g. Kravchuk Polynomials, see Atakishiyeva et al. [2014]).

To finalize the chapter on symmetry, we would like to also analyze gauge symmetry in our framework. We could implement the techniques of the lattice gauge theory community to see, whether corrected gauge Bosons behave different.

Another very interesting topic for future research is renormalization. This is especially interesting for us as it is directly connected to the discretization. Not unexpectedly, we already found a lot of traces of the divergences of the continuous theory. A lot of the quantities diverge for small spacing, but interestingly, some of them diverge differently. It turned out that the two discretization methods considered in this work are a good tool to analyze this and we believe that we can find some interesting physics behind these observations.

Another important difficulty of QED is defining the ground state. We are still not sure, how a QED ground state with non-diverging continuum limit would look like in our approach. To investigate this phenomenon deeper, we could try to implement time-dependence and perform imaginary time-propagation. This is a typical tool in other communities [Pang, 1997].

Also the analysis of electron and positron states appears possible: we could implement different techniques to differentiate between electrons and positrons and analyze their interaction. Especially the non-locality of pure electron or positron states could be investigated.

A very fruitful aspect of our model is its capability to visualize the complete Fock space of the theory also under variation of parameters, which allows for the investigation of limits

to other theories. The quantitative comparisons of analytical limits could be added to the qualitatively good results from section 5.2. For example, we could implement the non-relativistic Pauli Hamiltonian in our code to see whether the QED-Hamiltonian converges to it for $C \to \infty$. Also higher order corrections could be added.

Analyzing the Fock space of the limit theories is of course a promising task by itself.

Finally, we want to mention that our approach allows for arbitrary coordinate choice. Although we presented it here in real-space, we can do the same in momentum or any other space. It could also be interesting to deeper investigate the choice of coordinates within a certain space, for example exploiting the full Minkowski space and implement lightcone-coordinates. This is a typical tool for relativistic theories, and allows among others for a very easy definition of the ground state Brodsky et al. [1998].

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A Derivation of the Discretized Hamiltonian

For further usage and completeness, the derivation of all terms of the Hamiltonian is shown here explicitly. In the first part, the derivation is shown with examples for finite-differences and the Fourier method, respectively. In the second part, the terms are written-out and in the third part the specific 1D-1-mode model is shown.

A.1 Derivation of the Terms one by one

A.1.1 Mass Term H_{mass}

$$\psi^+ \mathcal{H}_{mass}\, \psi = m \sum_{\vec{r}_n, \vec{r}'_n} \underbrace{\sum_{\lambda,\lambda'} \vec{e}_\lambda \, \underline{\beta} \, \vec{e}_{\lambda'}}_{=(1,1,-1,-1)^T \equiv \vec{\beta}} \hat{c}^+_{\lambda,\vec{r}_n} \hat{c}_{\lambda',\vec{r}'_n} \underbrace{\Theta^3_{\vec{r}_n}(\vec{r})\, \Theta^3_{\vec{r}_n\,'}(\vec{r})}_{\int \mathrm{d}^3 r \to \delta_{\vec{r}_n \vec{r}_n\,'}}$$

$$H_{mass} = m \sum_{\vec{r}_n} \sum_{\lambda} \beta_\lambda \, \hat{c}^+_{\lambda,\vec{r}_n} \hat{c}_{\lambda,\vec{r}_n}$$

A.1.2 Kinetic Term H_{kin}

$$\psi^+ \mathcal{H}_{kin}\, \psi = -\mathbf{i}\hbar\, \psi^+ \underline{\alpha_i}\, \partial_i\, \psi = \mathcal{H}_{kin,x} + \mathcal{H}_{kin,y} + \mathcal{H}_{kin,z}$$

Finite Differences

$$\begin{aligned}
\mathcal{H}_{kin,x} &= -\mathbf{i}\hbar \sum_{\vec{r}_n, \vec{r}'_n} \underbrace{\sum_{\lambda,\lambda'} \hat{c}^+_{\lambda,\vec{r}_n} \, \vec{e}_\lambda \, \underline{\alpha_x} \, \vec{e}_{\lambda'} \, \hat{c}_{\lambda',\vec{r}'_n}}_{\equiv \mathcal{A}_x} \underbrace{\Theta^3_{\vec{r}_n}(\vec{r})\, \partial_x \Theta^3_{\vec{r}_n\,'}(\vec{r})}_{\equiv T_x} \\
&\to \int \mathrm{d}^3 r T_x = \frac{1}{2\Delta x} \left(\delta_{x_n x'_{n+1}} \delta_{y_n y'_n} \delta_{z_n z'_n} - \delta_{x_n x'_{n-1}} \delta_{y_n y'_n} \delta_{z_n z'_n} \right) \\
&\to \mathcal{A}_x = e_1\, \delta_{\lambda 1} \delta_{\lambda' 4} + e_2\, \delta_{\lambda 2} \delta_{\lambda' 3} + e_3\, \delta_{\lambda 3} \delta_{\lambda' 2} + e_2\, \delta_{\lambda 4} \delta_{\lambda' 1} \\
&\equiv \sum_\lambda \mathcal{H}_{kin,x,\lambda}
\end{aligned}$$

From these 4 terms exemplary the first is:

$$H_{kin,x,1} = -\frac{\mathbf{i}\hbar}{2\Delta x} \sum_{\vec{r}_n} \left(c^+_{1,\vec{r}_n} c_{4,x_{n+1} y_n z_n} - c^+_{1,\vec{r}_n} c_{4,x_{n-1} y_n z_n} \right)$$

The rest follows just by changing indices according to $\mathcal{A}_x$. For the x and y component just the respective delta symbols will be listed:

$$\int \mathrm{d}^3 r T_y = \frac{1}{2\Delta y}\left(\delta_{x_n x'_n}\delta_{y_n y'_{n+1}}\delta_{z_n z'_n} - \delta_{x_n x'_n}\delta_{y_n y'_{n-1}}\delta_{z_n z'_n}\right)$$
$$\mathcal{A}_y = e_1\,\delta_{\lambda 1}\delta_{\lambda' 4} + e_2\,\delta_{\lambda 2}\delta_{\lambda' 3} - e_3\,\delta_{\lambda 3}\delta_{\lambda' 2} - e_4\,\delta_{\lambda 4}\delta_{\lambda' 1}$$
$$\int \mathrm{d}^3 r T_z = \frac{\mathbf{i}}{2\Delta z}\left(\delta_{x_n x'_n}\delta_{y_n y'_n}\delta_{z_n z'_{n+1}} - \delta_{x_n x'_n}\delta_{y_n y'_n}\delta_{z_n z'_{n-1}}\right)$$
$$\mathcal{A}_z = e_1\,\delta_{\lambda 1}\delta_{\lambda' 3} + e_2\,\delta_{\lambda 2}\delta_{\lambda' 4} + e_3\,\delta_{\lambda 3}\delta_{\lambda' 1} + e_4\,\delta_{\lambda 4}\delta_{\lambda' 2}$$

Fourier-Method

$$\mathcal{H}_{kin,x} = -\mathbf{i}\hbar c \sum_{\vec{r}_n,\vec{r}'_n} \underbrace{\sum_{\lambda,\lambda'} \hat{c}^+_{\lambda,\vec{r}_n}\,\vec{e}_\lambda\,\underline{\alpha_x}\,\vec{e}_{\lambda'}\,\hat{c}_{\lambda',\vec{r}'_n}}_{\equiv \mathcal{A}_x \to \text{like before}} \underbrace{\Theta^3_{\vec{r}_n}(\vec{r})\,\partial_x \Theta^3_{\vec{r}_n\,'}(\vec{r})}_{\equiv T_x}$$
$$\to \int \mathrm{d}^3 r T_x = -\mathbf{i}\hbar \sum_{m=1}^{N_x} D_{x_n,x_m}\delta_{x_m x'_n}\delta_{y_n y'_n}\delta_{z_n z'_n}$$
$$\equiv \sum_\lambda \mathcal{H}_{kin,x,\lambda}$$
$$H_{kin,x,1} = -\mathbf{i}\hbar c \sum_{\vec{r}_n} c^+_{1,\vec{r}_n} \sum_{m=1}^{N_x} D_{x_n,x_m}\,c_{4,x_m y_n z_n}$$

A.1.3 Interaction Term H_{int}

$$\psi^+\,\mathcal{H}_{int}\,\psi = -e\psi^+\,\underline{\alpha}_i\,A_i\,\psi = \mathcal{H}_{int,x} + \mathcal{H}_{int,y} + \mathcal{H}_{int,z}$$
$$\mathcal{H}_{int,x} = -e \sum_{\vec{r}_n,\vec{r}'_n} \underbrace{\sum_{\lambda,\lambda'} \hat{c}^+_{\lambda,\vec{r}_n}\,\vec{e}_\lambda\,\underline{\alpha_x}\,\vec{e}_{\lambda'}\,\hat{c}_{\lambda',\vec{r}'_n}}_{=\mathcal{A}_x \text{ like in the kinetic case}} \underbrace{\Theta^3_{\vec{r}_n}(\vec{r})\,A_x \Theta^3_{\vec{r}_n\,'}(\vec{r})}_{\int \mathrm{d}^3 r \to A_{x,\vec{r}_n}\,\delta_{\vec{r}_n \vec{r}_n\,'}}$$
$$\equiv \sum_\lambda \mathcal{H}_{int,x,\lambda}$$

Note that the order of $\vec{A}$ and ψ was changed, which is possible as both operators access a different part of the Hilbert space. Again only the first term is presented exemplary, the rest follows straightforward:

$$H_{int,x,1} = -\frac{e}{\sqrt{2}} \sum_{\vec{r}_n} \left(c^+_{1,\vec{r}_n} c_{4,\vec{r}_n}\right)\left(\hat{a}^+_{1,\vec{r}_n} + \hat{a}_{1,\vec{r}_n}\right)$$

A.1.4 Magnetic Part of the EM Term $H_{EM,M}$

$$\begin{aligned}\mathcal{H}_{EM,M} &= \frac{\epsilon_0}{2}\left(\nabla\times\vec{A}\right)\left(\nabla\times\vec{A}\right) \overset{\substack{Lagrange\\Identity}}{=} \frac{\epsilon_0}{2}\left(\Delta\vec{A}^2-\left(\nabla\cdot\vec{A}\right)\left(\nabla\cdot\vec{A}\right)\right)\\ &= \frac{\epsilon_0}{2}\left(\partial_i\partial_i A_j A_j-\partial_i A_j\partial_j A_i\right)\\ &= \frac{\epsilon_0}{2}\left(\partial_i\partial_i\left(A_j\right)A_j+A_j\partial_i\partial_i\left(A_j\right)-\partial_i\left(A_j\right)\partial_j A_i-A_j\partial_i\partial_j A_i\right)\end{aligned}$$

There are three different types of terms: $\partial_i A_j, \partial_i\partial_j A_j, \partial_i\partial_i A_j A_j$. For each of them, one example will be shown explicitly in the following:

$$\begin{aligned}\left(A_2(\vec{r})\right)^2 &= \frac{1}{2}\sum_{\vec{r}_n\vec{r}'_n}^{\vec{N}}\vec{e}_y\vec{e}_y\left(\hat{a}^+_{2,\vec{r}_n}+\hat{a}_{2,\vec{r}_n}\right)\left(\hat{a}^+_{2,\vec{r}'_n}+\hat{a}_{2,\vec{r}'_n}\right)\Theta^3_{\vec{r}_n}\Theta^3_{\vec{r}'_n}\\ &= \frac{1}{2}\sum_{\vec{r}_n\vec{r}'_n}^{\vec{N}}\Big(\hat{a}^+_{2,\vec{r}_n}\hat{a}^+_{2,\vec{r}'_n}+\hat{a}^+_{2,\vec{r}_n}\hat{a}_{2,\vec{r}'_n}+\\ &\quad+\hat{a}_{2,\vec{r}_n}\hat{a}^+_{2,\vec{r}'_n}+\hat{a}_{2,\vec{r}_n}\hat{a}_{2,\vec{r}'_n}\Big)\Theta^3_{\vec{r}_n}\Theta^3_{\vec{r}'_n}\\ &\equiv A^2_{2,++}+A^2_{2,+0}+A^2_{2,0+}+A^2_{2,00}\end{aligned}$$

Finite Differences

$$\partial_x^2\left(A_{2,++}\right)A_{2,++} = \frac{1}{2}\sum_{\vec{r}_n\vec{r}'_n}^{\vec{N}}\left(\hat{a}^+_{2,\vec{r}_n}\hat{a}^+_{2,\vec{r}'_n}\right)\underbrace{\partial_x^2\Theta^3_{\vec{r}_n}\Theta^3_{\vec{r}'_n}}_{\int \mathrm{d}^3r\to\frac{1}{\Delta x^2}\left(\delta_{\vec{r}_n,x'_{n-1}y'_nz'_n}+\delta_{\vec{r}_n,x'_{n+1}y'_nz'_n}-2\delta_{\vec{r}_n,\vec{r}'_n}\right)}$$

$$\begin{aligned}\int\partial_x^2\left(A_{2,++}\right)A_{2,++}\mathrm{d}^3r &= \frac{1}{2\Delta_x^2}\sum_{\vec{r}_n}^{\vec{N}}\Big(\hat{a}^+_{2,\vec{r}_n}\hat{a}^+_{2,x_{n-1}y_nz_n}+\\ &\quad+\hat{a}^+_{2,\vec{r}_n}\hat{a}^+_{2,x_{n+1}y_nz_n}-2\,\hat{a}^+_{2,\vec{r}_n}\hat{a}^+_{2,\vec{r}_n}\Big)\end{aligned}$$

The other terms follow by dropping the dagger for the first, the second or both operators, respectively.
The second part $A_j\partial_i\partial_i\left(A_j\right)$ is the same with the order of the two operators exchanged. As operators commute for different sites, the terms just double:

$$\begin{aligned}\int\partial_x^2\left(A_{2,++}\right)A_{2,++}+A_{2,++}\partial_x^2\left(A_{2,++}\right)\mathrm{d}^3r &= \frac{1}{\Delta_x^2}\sum_{\vec{r}_n}^{\vec{N}}\Big(\hat{a}^+_{2,\vec{r}_n}\hat{a}^+_{2,x_{n-1}y_nz_n}+\\ &\quad+\hat{a}^+_{2,\vec{r}_n}\hat{a}^+_{2,x_{n+1}y_nz_n}-2\,\hat{a}^+_{2,\vec{r}_n}\hat{a}^+_{2,\vec{r}_n}\Big)\end{aligned}$$

For the other two terms follows:

$$\partial_x\partial_y A_2 = \frac{1}{\sqrt{2}}\sum_{\vec{r}_n}^{\vec{N}}\left(\hat{a}^+_{2,\vec{r}_n}+\hat{a}_{2,\vec{r}'_n}\right)\underbrace{\partial_x\partial_y\Theta^3_{\vec{r}_n}}$$

$$\rightarrow \tfrac{1}{4\Delta x\Delta y}\big(\Theta_{x_{n+1}}\Theta_{y_{n+1}}\Theta_{z_n}-\Theta_{x_{n-1}}\Theta_{y_{n+1}}\Theta_{z_n}-\Theta_{x_{n+1}}\Theta_{y_{n-1}}\Theta_{z_n}+\Theta_{x_{n-1}}\Theta_{y_{n-1}}\Theta_{z_n}\big)$$

$$\partial_x A_2 = \frac{1}{\sqrt{2}}\sum_{\vec{r}_n}^{\vec{N}}\left(\hat{a}^+_{2,\vec{r}_n}+\hat{a}_{2,\vec{r}'_n}\right)\underbrace{\partial_x\Theta^3_{\vec{r}_n}}$$

$$\rightarrow \tfrac{1}{2\Delta x}\big(\Theta_{x_{n+1}}\Theta_{y_n}\Theta_{z_n}-\Theta_{x_{n-1}}\Theta_{y_n}\Theta_{z_n}\big)$$

The explicit terms thus are:

$$\partial_x\left(A_1\right)\partial_y A_2 = \frac{1}{2}\sum_{\vec{r}_n,\vec{r}'_n}^{\vec{N}}\underbrace{\left(\hat{a}^+_{1,\vec{r}_n}+\hat{a}_{1,\vec{r}_n}\right)\left(\hat{a}^+_{2,\vec{r}'_n}+\hat{a}_{2,\vec{r}'_n}\right)}_{\mathcal{A}_{12}}\underbrace{\partial_x\Theta^3_{\vec{r}_n}\partial_y\Theta^3_{\vec{r}'_n}}_{\mathcal{T}_{xy}}$$

$$\rightarrow\mathcal{A}_{12}=\hat{a}^+_{1,\vec{r}_n}\,\hat{a}^+_{2,\vec{r}'_n}+\hat{a}^+_{1,\vec{r}_n}\,\hat{a}_{2,\vec{r}'_n}+\hat{a}_{1,\vec{r}_n}\,\hat{a}^+_{2,\vec{r}'_n}+\hat{a}_{1,\vec{r}_n}\,\hat{a}_{2,\vec{r}'_n}$$

$$\rightarrow\mathcal{T}_{xy}=\tfrac{1}{2\Delta x}\big(\Theta_{x_{n+1}}\Theta_{y_n}\Theta_{z_n}-\Theta_{x_{n-1}}\Theta_{y_n}\Theta_{z_n}\big)\tfrac{1}{2\Delta y}\left(\Theta_{x'_n}\Theta_{y'_{n+1}}\Theta_{z'_n}-\Theta_{x'_n}\Theta_{y'_{n-1}}\Theta_{z'_n}\right)$$

$$\int \mathrm{d}^3r\mathcal{T}_{xy}=\tfrac{1}{4\Delta x\Delta y}\Big(\delta_{x_{n+1}x'_n}\delta_{y_ny'_{n+1}}\delta_{z_nz'_n}-\delta_{x_{n-1}x'_n}\delta_{y_ny'_{n+1}}\delta_{z_nz'_n}-\delta_{x_{n+1}x'_n}\delta_{y_ny'_{n-1}}\delta_{z_nz'_n}+\delta_{x_{n-1}x'_n}\delta_{y_ny'_{n-1}}\delta_{z_nz'_n}\Big)$$

$$\equiv R_{++}+R_{+0}+R_{0+}+R_{00}$$

$$R_{++} = \frac{1}{8\Delta_x\Delta_y}\sum_{\vec{r}_n}^{\vec{N}}\hat{a}^+_{1,x_{n+1}y_nz_n}\,\hat{a}^+_{2,x_ny_{n+1}z_n}-\hat{a}^+_{1,x_{n-1}y_nz_n}\,\hat{a}^+_{2,x_ny_{n+1}z_n}-\hat{a}^+_{1,x_{n+1}y_nz_n}\,\hat{a}^+_{2,x_ny_{n-1}z_n}+\hat{a}^+_{1,x_{n-1}y_nz_n}\,\hat{a}^+_{2,x_ny_{n-1}z_n}$$

$$A_1\partial_x\partial_y A_2 = \frac{1}{2}\sum_{\vec{r}_n,\vec{r}'_n}^{\vec{N}}\underbrace{\left(\hat{a}^+_{1,\vec{r}_n}+\hat{a}_{1,\vec{r}_n}\right)\left(\hat{a}^+_{2,\vec{r}'_n}+\hat{a}_{2,\vec{r}'_n}\right)}_{\mathcal{A}_{12}}\underbrace{\Theta^3_{\vec{r}_n}\partial_x\partial_y\Theta^3_{\vec{r}'_n}}_{\mathcal{T}_{-xy}}$$

$$\rightarrow\mathcal{A}_{xy}\rightarrow\text{like above}$$

$$\rightarrow\mathcal{T}_{-xy}=\tfrac{1}{4\Delta x\Delta y}\Theta_{x_n}\Theta_{y_n}\Theta_{z_n}\left(\Theta_{x'_{n+1}}\Theta_{y'_{n+1}}\Theta_{z'_n}-\Theta_{x'_{n-1}}\Theta_{y'_{n+1}}\Theta_{z'_n}-\Theta_{x'_{n+1}}\Theta_{y'_{n-1}}\Theta_{z'_n}+\Theta_{x'_{n-1}}\Theta_{y'_{n-1}}\Theta_{z'_n}\right)$$

$$\int \mathrm{d}^3r\mathcal{T}_{-xy}=\tfrac{1}{4\Delta x\Delta y}\Big(\delta_{x_nx'_{n+1}}\delta_{y_ny'_{n+1}}\delta_{z_nz'_n}-\delta_{x_nx'_{n-1}}\delta_{y_ny'_{n+1}}\delta_{z_nz'_n}-\delta_{x_nx'_{n+1}}\delta_{y_ny'_{n-1}}\delta_{z_nz'_n}$$

$$
\begin{aligned}
&\qquad\qquad +\delta_{x_n x'_{n-1}}\delta_{y_n y'_{n-1}}\delta_{z_n z'_n}\Big) \\
&\equiv S_{++} + S_{+0} + S_{0+} + S_{00} \\
S_{++} &= \frac{1}{8\Delta_x\Delta_y}\sum_{\vec{r}_n}^{\vec{N}} \hat{a}^+_{1,\vec{r}_n}\,\hat{a}^+_{2,x_{n+1}y_{n+1}z_n} - \hat{a}^+_{1,\vec{r}_n}\,\hat{a}^+_{2,x_{n-1}y_{n+1}z_n} \\
&\qquad - \hat{a}^+_{1,\vec{r}_n}\,\hat{a}^+_{2,x_{n+1}y_{n-1}z_n} + \hat{a}^+_{1,\vec{r}_n}\,\hat{a}^+_{2,x_{n-1}y_{n-1}z_n}
\end{aligned}
$$

Fourier-Method Let us consider the first two terms:

$$
\partial_x^2\left(A_{2,+o}\right)A_{2,+o} = \frac{1}{2}\sum_{\vec{r}_n\vec{r}''_n}^{\vec{N}}\left(\hat{a}^+_{2,\vec{r}_n}\hat{a}_{2,\vec{r}''_n}\right)\underbrace{\partial_x^2\Theta^3_{\vec{r}_n}\Theta^3_{\vec{r}''_n}}_{\int \mathrm{d}^3r \to \sum_{m=1}^{N_i} L_{x_n,x_m}\delta_{x_m x'_n}\delta_{y_n y'_n}\delta_{z_n z'_n}}
$$

$$
\int \partial_x^2\left(A_{2,+o}\right)A_{2,+o}\mathrm{d}^3r = \frac{1}{2}\sum_{\vec{r}_n}^{\vec{N}}\sum_{m=1}^{N_x} L_{x_n,x_m}\hat{a}^+_{2,x_m y_n z_n}\hat{a}_{2,\vec{r}_n}
$$

The second term is equivalent to the first up to a commutation error (that does not arise in the finite differences case):

$$
\begin{aligned}
\int A_{2,+o}\partial_x^2\left(A_{2,+o}\right)\mathrm{d}^3r &= \frac{1}{2}\sum_{\vec{r}_n}^{\vec{N}}\hat{a}^+_{2,\vec{r}_n}\sum_{m=1}^{N_x} L_{x_n,x_m}\hat{a}_{2,x_m y_n z_n} \\
&= \frac{s}{2}\sum_{\vec{r}_n}^{\vec{N}}\sum_{m=1}^{N_x} L_{x_n,x_m}\hat{a}_{2,x_m y_n z_n}\hat{a}^+_{2,\vec{r}_n} + r \\
\text{with } r &= \begin{cases} N_x+N_y+N_z & \text{for o+} \\ -(N_x+N_y+N_z) & \text{for +o} \\ 0 & \text{for ++,oo} \end{cases} \\
\text{and } s &= \begin{cases} -1 & \text{for o+} \\ 1 & \text{else} \end{cases} \\
\text{where we used: } & a_i a_j^+ - a_j^+ a_i = \delta_{ij}
\end{aligned}
$$

So we have for both terms together:

$$
\begin{aligned}
++ &\to \sum_{\vec{r}_n}^{\vec{N}}\sum_{m=1}^{N_x} L_{x_n,x_m}\hat{a}^+_{2,x_m y_n z_n}\hat{a}^+_{2,\vec{r}_n} \\
2(+o) &\to \sum_{\vec{r}_n}^{\vec{N}}\sum_{m=1}^{N_x} L_{x_n,x_m}\hat{a}^+_{2,x_m y_n z_n}\hat{a}_{2,\vec{r}_n} + \sum_{\vec{r}_n}^{\vec{N}}\sum_{m=1}^{N_x} L_{x_n,x_m}\hat{a}_{2,x_m y_n z_n}\hat{a}^+_{2,\vec{r}_n} - (N_x+N_y+N_z)
\end{aligned}
$$

$$2(o+) \rightarrow \sum_{\vec{r}_n}^{\vec{N}} \sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}_{2,x_m y_n z_n} \hat{a}^+_{2,\vec{r}_n} - \sum_{\vec{r}_n}^{\vec{N}} \sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}^+_{2,x_m y_n z_n} \hat{a}_{2,\vec{r}_n} + (N_x + N_y + N_z)$$

$$oo \rightarrow \sum_{\vec{r}_n}^{\vec{N}} \sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}_{2,x_m y_n z_n} \hat{a}_{2,\vec{r}_n}$$

We see that the commutation terms cancel each other and that the one of the mixed terms that contains the derivative of the creation operator becomes zero:

$$\int \partial_x^2 A_i^2 \mathrm{d}^3 r = \sum_{\vec{r}_n}^{\vec{N}} \left(\sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}^+_{i,x_m y_n z_n} \hat{a}^+_{i,\vec{r}_n} + \sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}_{i,x_m y_n z_n} \hat{a}^+_{i,\vec{r}_n} + \sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}_{i,x_m y_n z_n} \hat{a}_{iu,\vec{r}_n} \right)$$

For the other two terms follows:

$$\partial_x \partial_y A_2 = \frac{1}{2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}^+_{i,\vec{r}_n} + \hat{a}_{i,\vec{r}_n} \right) \underbrace{\partial_x \partial_y \Theta^3_{\vec{r}_n}}_{\rightarrow \sum_{m=1}^{N_x} D_{x_n,x_m} \Theta_{x_m} \sum_{m=1}^{N_y} D_{y_n,y_m} \Theta_{y_m} \Theta_{z_n}}$$

$$\partial_x A_2 = \frac{1}{\sqrt{2}} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}^+_{2,\vec{r}_n} + \hat{a}_{2,\vec{r}'_n} \right) \underbrace{\partial_x \Theta^3_{\vec{r}_n}}_{\rightarrow \sum_{m=1}^{N_x} D_{x_n,x_m} \Theta_{x_m} \Theta_{y_n} \Theta_{z_n}}$$

Now we can construct all the explicit terms of the magnetic part:

$$\partial_x (A_1) \, \partial_y A_2 = \frac{1}{2} \sum_{\vec{r}_n,\vec{r}'_n}^{\vec{N}} \underbrace{\left(\hat{a}^+_{1,\vec{r}_n} + \hat{a}_{1,\vec{r}_n} \right) \left(\hat{a}^+_{2,\vec{r}'_n} + \hat{a}_{2,\vec{r}'_n} \right)}_{\mathcal{A}_{12}} \underbrace{\partial_x \Theta^3_{\vec{r}_n} \partial_y \Theta^3_{\vec{r}'_n}}_{\mathcal{T}_{xy}}$$

$$\rightarrow \mathcal{A}_{xy} = \hat{a}^+_{1,\vec{r}_n} \hat{a}^+_{2,\vec{r}'_n} + \hat{a}^+_{1,\vec{r}_n} \hat{a}_{2,\vec{r}'_n} + \hat{a}_{1,\vec{r}_n} \hat{a}^+_{2,\vec{r}'_n} + \hat{a}_{1,\vec{r}_n} \hat{a}_{2,\vec{r}'_n}$$

$$\rightarrow \mathcal{T}_{xy} = \sum_{m=1}^{N_x} D_{x_n,x_m} \Theta_{x_m} \Theta_{x'_n} \Theta_{y_n} \sum_{m=1}^{N_y} D_{y_n,y'_m} \Theta_{y'_m} \Theta_{z_n} \Theta_{z'_n}$$

$$\int \mathrm{d}^3 r \mathcal{T}_{xy} = \sum_{m=1}^{N_x} D_{x_n,x_m} \delta_{x_m,x'_n} \sum_{m=1}^{N_y} D_{y'_n,y'_m} \delta_{y_n,y'_m} \delta_{z_n z'_n}$$

$$\equiv R_{++} + R_{+o} + R_{o+} + R_{oo}$$

$$\rightarrow R_{+o} = \frac{1}{2} \sum_{\vec{r}_n}^{\vec{N}} \sum_{m=1}^{N_x} D_{x_n,x_m} \hat{a}^+_{1,x_m y_n z_n} \sum_{m=1}^{N_y} D_{y_n,y_m} \hat{a}_{2,x_n y_m z_n}$$

And for the last type of term:

$$A_1\partial_x\partial_y A_2 = \frac{1}{2}\sum_{\vec{r}_n,\vec{r}'_n}^{\vec{N}} \underbrace{\left(\hat{a}^+_{1,\vec{r}_n} + \hat{a}_{1,\vec{r}_n}\right)\left(\hat{a}^+_{2,\vec{r}'_n} + \hat{a}_{2,\vec{r}'_n}\right)}_{\mathcal{A}_{12}} \underbrace{\Theta^3_{\vec{r}_n}\partial_x\partial_y\Theta^3_{\vec{r}'_n}}_{\mathcal{T}^*_{xy}}$$

$$\rightarrow \mathcal{A}_{xy} \rightarrow \text{like above}$$

$$\rightarrow \mathcal{T}^*_{xy} = \Theta_{x_n}\sum_{m=1}^{N_x} D_{x'_n,x'_m}\Theta_{x'_m}\Theta_{y_n}\sum_{m=1}^{N_y} D_{y'_n,y'_m}\Theta_{y'_m}\Theta_{z_n}\Theta_{z'_n}$$

$$\int \mathrm{d}^3r\mathcal{T}^*_{xy} = \sum_{m=1}^{N_x} D_{x'_n,x'_m}\delta_{x_n,x'_m}\sum_{m=1}^{N_y} D_{y'_n,y'_m}\delta_{y_n,y'_m}\delta_{z_nz'_n}$$

$$\equiv S_{++} + S_{+0} + S_{0+} + S_{00}$$

$$\rightarrow S_{+o} = \frac{1}{2}\sum_{\vec{r}_n}^{\vec{N}} \hat{a}^+_{1,x_ny_nz_n}\sum_{k=1}^{N_x} D_{x_n,x_k}\sum_{m=1}^{N_y} D_{y_n,y_m}\hat{a}_{2,x_ky_mz_n}$$

A.1.5 Electric Part of the EM-Term $H_{EM,E}$

As we defined already $\vec{E}$ as the conjugate momentum to $\vec{A}$, it is comparatively easy to calculate this last part of the Hamiltonian:

$$\mathcal{H}_{EM,E} = \frac{1}{2}\vec{E}^2 = \frac{1}{2}\left(E_1^2 + E_2^2 + E_3^2\right)$$

$$E_1^2 = \frac{\mathbf{i}^2}{2}\sum_{\vec{r}_n,\vec{r}'_n}^{\vec{N}} \left(\hat{a}_{1,\vec{r}_n} - \hat{a}^+_{1,\vec{r}_n}\right)\left(\hat{a}_{1,\vec{r}_n\,\prime} - \hat{a}^+_{1,\vec{r}_n\,\prime}\right) \underbrace{\Theta^3_{\vec{r}_n}(\vec{r})\,\Theta^3_{\vec{r}_n\,\prime}(\vec{r})}_{\int \mathrm{d}^3r \rightarrow \delta_{\vec{r}_n\vec{r}_n\,\prime}}$$

$$H_{EM,E,1} = \frac{1}{2}\sum_{\vec{r}_n}^{\vec{N}} -\hat{a}_{1,\vec{r}_n}\hat{a}_{1,\vec{r}_n} + \hat{a}^+_{1,\vec{r}_n}\hat{a}_{1,\vec{r}_n} + \hat{a}_{1,\vec{r}_n}\hat{a}^+_{1,\vec{r}_n} - \hat{a}^+_{1,\vec{r}_n}\hat{a}^+_{1,\vec{r}_n}$$

A.2 The Full Hamiltonian

All put together we have:

Finite differences

$$H_{Dirac} = H_{mass} + H_{kin}$$

$$= m\sum_{\vec{r}_n}\sum_{\lambda}\beta_\lambda\,\hat{c}^+_{\lambda,\vec{r}_n}\,\hat{c}_{\lambda,\vec{r}'_n}$$

$$-\frac{\mathbf{i}\hbar c}{2\Delta x}\sum_{\vec{r}_n}\left(c^+_{1,\vec{r}_n}c_{4,x_{n+1}y_nz_n} - c^+_{1,\vec{r}_n}c_{4,x_{n-1}y_nz_n}\right)$$

$$
\begin{aligned}
&- \frac{\mathbf{i}\hbar c}{2\Delta x} \sum_{\vec{r}_n} \left(c^+_{2,\vec{r}_n} c_{3,x_{n+1}y_n z_n} - c^+_{2,\vec{r}_n} c_{3,x_{n-1}y_n z_n} \right) \\
&- \frac{\mathbf{i}\hbar c}{2\Delta x} \sum_{\vec{r}_n} \left(c^+_{3,\vec{r}_n} c_{2,x_{n+1}y_n z_n} - c^+_{1,\vec{r}_n} c_{4,x_{n-1}y_n z_n} \right) \\
&- \frac{\mathbf{i}\hbar c}{2\Delta x} \sum_{\vec{r}_n} \left(c^+_{4,\vec{r}_n} c_{1,x_{n+1}y_n z_n} - c^+_{4,\vec{r}_n} c_{1,x_{n-1}y_n z_n} \right) \\
&+ H_{kin,y} + H_{kin,z}
\end{aligned}
$$

Fourier Method

$$
\begin{aligned}
H_{Dirac} &= H_{mass} + H_{kin} \\
&= mc^2 \sum_{\vec{r}_n} \sum_{\lambda} \beta_\lambda \, \hat{c}^+_{\lambda,\vec{r}_n} \, \hat{c}_{\lambda,\vec{r}_n} \\
&- \mathbf{i}\hbar c \sum_{\vec{r}_n} c^+_{1,\vec{r}_n} \sum_{m=1}^{N_x} D_{x_n,x_m} \, c_{4,x_m y_n z_n} - \mathbf{i}\hbar c \sum_{\vec{r}_n} c^+_{2,\vec{r}_n} \sum_{m=1}^{N_x} D_{x_n,x_m} \, c_{3,x_m y_n z_n} \\
&- \mathbf{i}\hbar c \sum_{\vec{r}_n} c^+_{3,\vec{r}_n} \sum_{m=1}^{N_x} D_{x_n,x_m} \, c_{2,x_m y_n z_n} - \mathbf{i}\hbar c \sum_{\vec{r}_n} c^+_{4,\vec{r}_n} \sum_{m=1}^{N_x} D_{x_n,x_m} \, c_{1,x_m y_n z_n} \\
&+ H_{kin,y} + H_{kin,z}
\end{aligned}
$$

The interaction term does not involve derivatives, so there is only one version

$$
\begin{aligned}
H_{int} = &- \frac{e}{\sqrt{2}} \sum_{\vec{r}_n} \left(c^+_{1,\vec{r}_n} c_{4,\vec{r}_n} \right) \left(\hat{a}^+_{1,\vec{r}_n} + \hat{a}_{1,\vec{r}_n} \right) - \frac{e}{\sqrt{2}} \sum_{\vec{r}_n} \left(c^+_{2,\vec{r}_n} c_{3,\vec{r}_n} \right) \left(\hat{a}^+_{1,\vec{r}_n} + \hat{a}_{1,\vec{r}_n} \right) \\
&- \frac{e}{\sqrt{2}} \sum_{\vec{r}_n} \left(c^+_{3,\vec{r}_n} c_{2,\vec{r}_n} \right) \left(\hat{a}^+_{1,\vec{r}_n} + \hat{a}_{1,\vec{r}_n} \right) - \frac{e}{\sqrt{2}} \sum_{\vec{r}_n} \left(c^+_{4,\vec{r}_n} c_{1,\vec{r}_n} \right) \left(\hat{a}^+_{1,\vec{r}_n} + \hat{a}_{1,\vec{r}_n} \right) \\
&+ \frac{e}{\sqrt{2}} \mathbf{i} \sum_{\vec{r}_n} \left(c^+_{1,\vec{r}_n} c_{4,\vec{r}_n} \right) \left(\hat{a}^+_{2,\vec{r}_n} + \hat{a}_{2,\vec{r}_n} \right) + \frac{e}{\sqrt{2}} \mathbf{i} \sum_{\vec{r}_n} \left(c^+_{2,\vec{r}_n} c_{3,\vec{r}_n} \right) \left(\hat{a}^+_{2,\vec{r}_n} + \hat{a}_{2,\vec{r}_n} \right) \\
&- \frac{e}{\sqrt{2}} \mathbf{i} \sum_{\vec{r}_n} \left(c^+_{3,\vec{r}_n} c_{2,\vec{r}_n} \right) \left(\hat{a}^+_{2,\vec{r}_n} + \hat{a}_{2,\vec{r}_n} \right) - \frac{e}{\sqrt{2}} \mathbf{i} \sum_{\vec{r}_n} \left(c^+_{4,\vec{r}_n} c_{1,\vec{r}_n} \right) \left(\hat{a}^+_{2,\vec{r}_n} + \hat{a}_{2,\vec{r}_n} \right) \\
&- \frac{e}{\sqrt{2}} \sum_{\vec{r}_n} \left(c^+_{1,\vec{r}_n} c_{3,\vec{r}_n} \right) \left(\hat{a}^+_{3,\vec{r}_n} + \hat{a}_{3,\vec{r}_n} \right) - \frac{e}{\sqrt{2}} \sum_{\vec{r}_n} \left(c^+_{2,\vec{r}_n} c_{4,\vec{r}_n} \right) \left(\hat{a}^+_{3,\vec{r}_n} + \hat{a}_{3,\vec{r}_n} \right) \\
&+ \frac{e}{\sqrt{2}} \sum_{\vec{r}_n} \left(c^+_{3,\vec{r}_n} c_{1,\vec{r}_n} \right) \left(\hat{a}^+_{3,\vec{r}_n} + \hat{a}_{3,\vec{r}_n} \right) + \frac{e}{\sqrt{2}} \sum_{\vec{r}_n} \left(c^+_{4,\vec{r}_n} c_{2,\vec{r}_n} \right) \left(\hat{a}^+_{3,\vec{r}_n} + \hat{a}_{3,\vec{r}_n} \right)
\end{aligned}
$$

Finally the em-field:

Finite Differences

$$
\begin{aligned}
H_{EM} = & \frac{\epsilon_0}{2\Delta x^2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}^+_{1,\vec{r}_n} \hat{a}^+_{1,x_{n-1}y_nz_n} + \hat{a}^+_{1,\vec{r}_n} \hat{a}^+_{1,x_{n+1}y_nz_n} - 2\, \hat{a}^+_{1,\vec{r}_n} \hat{a}^+_{1,\vec{r}_n} \right) \\
& + \frac{\epsilon_0}{2\Delta x^2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}^+_{1,\vec{r}_n} \hat{a}_{1,x_{n-1}y_nz_n} + \hat{a}^+_{1,\vec{r}_n} \hat{a}_{1,x_{n+1}y_nz_n} - 2\, \hat{a}^+_{1,\vec{r}_n} \hat{a}_{1,\vec{r}_n} + \right) \\
& + \frac{\epsilon_0}{2\Delta x^2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}_{1,\vec{r}_n} \hat{a}^+_{1,x_{n-1}y_nz_n} + \hat{a}_{1,\vec{r}_n} \hat{a}^+_{1,x_{n+1}y_nz_n} - 2\, \hat{a}_{1,\vec{r}_n} \hat{a}^+_{1,\vec{r}_n} \right) \\
& + \frac{\epsilon_0}{2\Delta x^2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}_{1,\vec{r}_n} \hat{a}_{1,x_{n-1}y_nz_n} + \hat{a}_{1,\vec{r}_n} \hat{a}_{1,x_{n+1}y_nz_n} - 2\, \hat{a}_{1,\vec{r}_n} \hat{a}_{1,\vec{r}_n} \right) \\
& + H_{A^2,dx,2} + H_{A^2,dx,3} \\
& + H_{A^2,dy} + H_{A^2,dz} \\
& + \frac{\epsilon_0}{16\Delta x^2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}^+_{1,x_{n+1}y_nz_n}\, \hat{a}^+_{1,x_{n+1}y_nz_n} - \hat{a}^+_{1,x_{n-1}y_nz_n}\, \hat{a}^+_{1,x_{n+1}y_nz_n} \right. \\
& \qquad \left. - \hat{a}^+_{1,x_{n+1}y_nz_n}\, \hat{a}^+_{1,x_{n-1}y_nz_n} + \hat{a}^+_{1,x_{n-1}y_nz_n}\, \hat{a}^+_{1,x_{n-1}y_nz_n} \right) \\
& + \frac{\epsilon_0}{16\Delta x^2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}^+_{1,x_{n+1}y_nz_n}\, \hat{a}_{1,x_{n+1}y_nz_n} - \hat{a}^+_{1,x_{n-1}y_nz_n}\, \hat{a}_{1,x_{n+1}y_nz_n} \right. \\
& \qquad \left. - \hat{a}^+_{1,x_{n+1}y_nz_n}\, \hat{a}_{1,x_{n-1}y_nz_n} + \hat{a}^+_{1,x_{n-1}y_nz_n}\, \hat{a}_{1,x_{n-1}y_nz_n} \right) \\
& + \frac{\epsilon_0}{16\Delta x^2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}_{1,x_{n+1}y_nz_n}\, \hat{a}^+_{1,x_{n+1}y_nz_n} - \hat{a}_{1,x_{n-1}y_nz_n}\, \hat{a}^+_{1,x_{n+1}y_nz_n} \right. \\
& \qquad \left. - \hat{a}_{1,x_{n+1}y_nz_n}\, \hat{a}^+_{1,x_{n-1}y_nz_n} + \hat{a}_{1,x_{n-1}y_nz_n}\, \hat{a}^+_{1,x_{n-1}y_nz_n} \right) \\
& + \frac{\epsilon_0}{16\Delta x^2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}_{1,x_{n+1}y_nz_n}\, \hat{a}_{1,x_{n+1}y_nz_n} - \hat{a}_{1,x_{n-1}y_nz_n}\, \hat{a}_{1,x_{n+1}y_nz_n} \right. \\
& \qquad \left. - \hat{a}_{1,x_{n+1}y_nz_n}\, \hat{a}_{1,x_{n-1}y_nz_n} + \hat{a}_{1,x_{n-1}y_nz_n}\, \hat{a}_{1,x_{n-1}y_nz_n} \right) \\
& + H_{A_{1,x}A_{2,y}} + H_{A_{1,x}A_{3,z}} + H_{A_{2,y}A_{1,x}} + H_{A_{2,y}A_{2,y}} + H_{A_{2,y}A_{3,z}} \\
& + H_{A_{3,z}A_{1,x}} + H_{A_{3,z}A_{2,y}} + H_{A_{3,z}A_{3,z}} \\
& + \frac{\epsilon_0}{4\Delta x^2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}^+_{1,\vec{r}_n}\, \hat{a}^+_{1,x_{n+1}y_nz_n} + \hat{a}^+_{1,\vec{r}_n}\, \hat{a}^+_{1,x_{n-1}y_nz_n} - 2\, \hat{a}^+_{1,\vec{r}_n} \hat{a}^+_{1,\vec{r}_n} \right) \\
& + \frac{\epsilon_0}{4\Delta x^2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}^+_{1,\vec{r}_n}\, \hat{a}_{1,x_{n+1}y_nz_n} + \hat{a}^+_{1,\vec{r}_n}\, \hat{a}_{1,x_{n-1}y_nz_n} - 2\, \hat{a}_{1,\vec{r}_n} \hat{a}^+_{1,\vec{r}_n} \right) \\
& + \frac{\epsilon_0}{4\Delta x^2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}_{1,\vec{r}_n}\, \hat{a}^+_{1,x_{n+1}y_nz_n} + \hat{a}_{1,\vec{r}_n}\, \hat{a}^+_{1,x_{n-1}y_nz_n} - 2\, \hat{a}_{1,\vec{r}_n} \hat{a}^+_{1,\vec{r}_n} \right)
\end{aligned}
$$

$$
\begin{aligned}
&+ \frac{\epsilon_0}{4\Delta x^2} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}_{1,\vec{r}_n} \hat{a}_{1,x_{n+1}y_nz_n} + \hat{a}_{1,\vec{r}_n} \hat{a}_{1,x_{n-1}y_nz_n} - 2\,\hat{a}_{1,\vec{r}_n}\hat{a}_{1,\vec{r}_n} \right) \\
&+ H_{A_1A_{2,xy}} + H_{A_1A_{3,xz}} + H_{A_2A_{1,yx}} + H_{A_2A_{2,yy}} + H_{A_2A_{3,yz}} \\
&+ H_{A_3A_{1,zx}} + H_{A_3A_{2,zy}} + H_{A_3A_{3,zz}} \\
&- \frac{\epsilon_0 c}{4} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}_{1,\vec{r}_n}\hat{a}_{1,\vec{r}_n} - \hat{a}^+_{1,\vec{r}_n}\hat{a}_{1,\vec{r}_n} - \hat{a}_{1,\vec{r}_n}\hat{a}^+_{1,\vec{r}_n} + \hat{a}^+_{1,\vec{r}_n}\hat{a}^+_{1,\vec{r}_n} \right) \\
&- \frac{\epsilon_0 c}{4} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}_{2,\vec{r}_n}\hat{a}_{2,\vec{r}_n} - \hat{a}^+_{2,\vec{r}_n}\hat{a}_{2,\vec{r}_n} - \hat{a}_{2,\vec{r}_n}\hat{a}^+_{2,\vec{r}_n} + \hat{a}^+_{2,\vec{r}_n}\hat{a}^+_{2,\vec{r}_n} \right) \\
&- \frac{\epsilon_0 c}{4} \sum_{\vec{r}_n}^{\vec{N}} \left(\hat{a}_{3,\vec{r}_n}\hat{a}_{3,\vec{r}_n} - \hat{a}^+_{3,\vec{r}_n}\hat{a}_{3,\vec{r}_n} - \hat{a}_{3,\vec{r}_n}\hat{a}^+_{3,\vec{r}_n} + \hat{a}^+_{3,\vec{r}_n}\hat{a}^+_{3,\vec{r}_n} \right)
\end{aligned}
$$

Fourier-Method

$$
\begin{aligned}
H_{M,A^2} &= \frac{\epsilon_0}{2}((\partial_i\partial_i A_j)A_j + A_j(\partial_i\partial_i A_j)) \\
&= \epsilon_0 \sum_{\vec{r}_n}^{\vec{N}} \left(\sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}^+_{1,x_m y_n z_n} \hat{a}^+_{1,\vec{r}_n} + \sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}_{1,x_m y_n z_n} \left(\hat{a}^+_{1,\vec{r}_n} + \hat{a}_{1,\vec{r}_n} \right) \right) \\
&+ \epsilon_0 \sum_{\vec{r}_n}^{\vec{N}} \left(\sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}^+_{2,x_m y_n z_n} \hat{a}^+_{2,\vec{r}_n} + \sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}_{2,x_m y_n z_n} \left(\hat{a}^+_{2,\vec{r}_n} + \hat{a}_{2,\vec{r}_n} \right) \right) \\
&+ \epsilon_0 \sum_{\vec{r}_n}^{\vec{N}} \left(\sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}^+_{3,x_m y_n z_n} \hat{a}^+_{3,\vec{r}_n} + \sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}_{3,x_m y_n z_n} \left(\hat{a}^+_{3,\vec{r}_n} + \hat{a}_{3,\vec{r}_n} \right) \right) \\
&+ H_{A^2,dy} + H_{A^2,dz}
\end{aligned}
$$

$$
\begin{aligned}
H_{M,dA_i dA_j} &= -\frac{\epsilon_0}{2}(\partial_i A_j)(\partial_j A_i) \\
&= -\frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \sum_{m=1}^{N_x} D_{x_n,x_m} \hat{a}^+_{1,x_m y_n z_n} \sum_{m=1}^{N_y} D_{x_n,x_m} \hat{a}^+_{1,x_m y_n z_n} \\
&- \frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \sum_{m=1}^{N_x} D_{x_n,x_m} \hat{a}^+_{1,x_m y_n z_n} \sum_{m=1}^{N_y} D_{x_n,x_m} \hat{a}_{1,x_m y_n z_n} \\
&- \frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \sum_{m=1}^{N_x} D_{x_n,x_m} \hat{a}_{1,x_m y_n z_n} \sum_{m=1}^{N_y} D_{x_n,x_m} \hat{a}^+_{1,x_m y_n z_n} \\
&- \frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \sum_{m=1}^{N_x} D_{x_n,x_m} \hat{a}_{1,x_m y_n z_n} \sum_{m=1}^{N_y} D_{x_n,x_m} \hat{a}_{1,x_m y_n z_n}
\end{aligned}
$$

$$+ H_{A_{2,dx}A_{1,dy}} + H_{A_{3,dx}A_{1,dz}} + H_{A_{1,dy}A_{2,dx}} + H_{A_{2,dy}A_{2,dy}} + H_{A_{3,dy}A_{2,z}}$$
$$+ H_{A_{1,dz}A_{3,x}} + H_{A_{2,dz}A_{3,dy}} + H_{A_{3,dz}A_{3,dz}}$$

$$\begin{aligned}
H_{M,A_i dd A_j} &= -\frac{\epsilon_0}{2} A_j(\partial_i \partial_j A_i) = -\frac{1}{2} A_j(\partial_j \partial_i A_i) \\
&= -\frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \hat{a}^+_{1,x_n y_n z_n} \sum_{k=1}^{N_x} D_{x_n,x_k} \sum_{m=1}^{N_x} D_{x_k,x_m} \hat{a}^+_{1,x_k y_n z_n} \\
&- \frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \hat{a}^+_{1,x_n y_n z_n} \sum_{k=1}^{N_x} D_{x_n,x_k} \sum_{m=1}^{N_x} D_{x_k,x_m} \hat{a}_{1,x_k y_n z_n} \\
&- \frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \hat{a}_{1,x_n y_n z_n} \sum_{k=1}^{N_x} D_{x_n,x_k} \sum_{m=1}^{N_x} D_{x_k,x_m} \hat{a}^+_{1,x_k y_n z_n} \\
&- \frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \hat{a}_{1,x_n y_n z_n} \sum_{k=1}^{N_x} D_{x_n,x_k} \sum_{m=1}^{N_x} D_{x_k,x_m} \hat{a}_{1,x_k y_n z_n} \\
&+ H_{A_1 A_{2,xy}} + H_{A_1 A_{3,xz}} + H_{A_2 A_{1,yx}} + H_{A_2 A_{2,yy}} + H_{A_2 A_{3,yz}} \\
&+ H_{A_3 A_{1,zx}} + H_{A_3 A_{2,zy}} + H_{A_3 A_{3,zz}}
\end{aligned}$$

$$\begin{aligned}
H_E = &\frac{\epsilon_0 c}{4} \sum_{\vec{r}_n}^{\vec{N}} \left(-\hat{a}_{1,\vec{r}_n} \hat{a}_{1,\vec{r}_n} + \hat{a}^+_{1,\vec{r}_n} \hat{a}_{1,\vec{r}_n} + \hat{a}_{1,\vec{r}_n} \hat{a}^+_{1,\vec{r}_n} - \hat{a}^+_{1,\vec{r}_n} \hat{a}^+_{1,\vec{r}_n} \right) \\
&+ \frac{\epsilon_0 c}{4} \sum_{\vec{r}_n}^{\vec{N}} \left(-\hat{a}_{2,\vec{r}_n} \hat{a}_{2,\vec{r}_n} + \hat{a}^+_{2,\vec{r}_n} \hat{a}_{2,\vec{r}_n} + \hat{a}_{2,\vec{r}_n} \hat{a}^+_{2,\vec{r}_n} - \hat{a}^+_{2,\vec{r}_n} \hat{a}^+_{2,\vec{r}_n} \right) \\
&+ \frac{\epsilon_0 c}{4} \sum_{\vec{r}_n}^{\vec{N}} \left(-\hat{a}_{3,\vec{r}_n} \hat{a}_{3,\vec{r}_n} + \hat{a}^+_{3,\vec{r}_n} \hat{a}_{3,\vec{r}_n} + \hat{a}_{3,\vec{r}_n} \hat{a}^+_{3,\vec{r}_n} - \hat{a}^+_{3,\vec{r}_n} \hat{a}^+_{3,\vec{r}_n} \right)
\end{aligned}$$

A.3 The 1D-1-Mode-Hamiltonian

To derive the model that was used throughout this work, let us consider spatial confinement in y and z direction, which means $N_y = N_z = 1$ and thus vanishing differential operators in y and z direction. It is also assumed, that the field has only one polarization mode (e.g. longitudinal photons). It follows:

Finite Differences

$$
\begin{aligned}
H_{pre} = {} & mc^2 \sum_{x_n} \sum_{\lambda} \beta_\lambda \, \hat{c}^+_{\lambda,x_n} \, \hat{c}_{\lambda,x'_n} \\
& - \frac{\mathbf{i}\hbar c}{2\Delta x} \sum_{x_n} \left(c^+_{1,x_n} c_{4,x_{n+1}} - c^+_{1,x_n} c_{4,x_{n-1}} \right) - \frac{\mathbf{i}\hbar c}{2\Delta x} \sum_{x_n} \left(c^+_{2,x_n} c_{3,x_{n+1}} - c^+_{2,x_n} c_{3,x_{n-1}} \right) \\
& - \frac{\mathbf{i}\hbar c}{2\Delta x} \sum_{x_n} \left(c^+_{3,x_n} c_{2,x_{n+1}} - c^+_{1,x_n} c_{4,x_{n-1}} \right) - \frac{\mathbf{i}\hbar c}{2\Delta x} \sum_{x_n} \left(c^+_{4,x_n} c_{1,x_{n+1}} - c^+_{4,x_n} c_{1,x_{n-1}} \right) \\
& - \frac{e}{\sqrt{2}} \sum_{x_n} \left(c^+_{1,x_n} c_{4,x_n} \right) \left(\hat{a}^+_{1,x_n} + \hat{a}_{1,x_n} \right) - \frac{e}{\sqrt{2}} \sum_{x_n} \left(c^+_{2,x_n} c_{3,x_n} \right) \left(\hat{a}^+_{1,x_n} + \hat{a}_{1,x_n} \right) \\
& - \frac{e}{\sqrt{2}} \sum_{x_n} \left(c^+_{3,x_n} c_{2,x_n} \right) \left(\hat{a}^+_{1,x_n} + \hat{a}_{1,x_n} \right) - \frac{e}{\sqrt{2}} \sum_{x_n} \left(c^+_{4,x_n} c_{1,x_n} \right) \left(\hat{a}^+_{1,x_n} + \hat{a}_{1,x_n} \right) \\
& + \frac{3\epsilon_0}{4\Delta x^2} \sum_{x_n} \left(\hat{a}^+_{1,x_n} \hat{a}^+_{1,x_{n-1}} + \hat{a}^+_{1,x_n} \hat{a}^+_{1,x_{n+1}} - 2\, \hat{a}^+_{1,x_n} \hat{a}^+_{1,x_n} \right) \\
& + \frac{3\epsilon_0}{4\Delta x^2} \sum_{x_n} \left(\hat{a}^+_{1,x_n} \hat{a}_{1,x_{n-1}} + \hat{a}^+_{1,x_n} \hat{a}_{1,x_{n+1}} - 2\, \hat{a}^+_{1,x_n} \hat{a}_{1,x_n} \right) \\
& + \frac{3\epsilon_0}{4\Delta x^2} \sum_{x_n} \left(\hat{a}_{1,x_n} \hat{a}^+_{1,x_{n-1}} + \hat{a}_{1,x_n} \hat{a}^+_{1,x_{n+1}} - 2\, \hat{a}_{1,x_n} \hat{a}^+_{1,x_n} \right) \\
& + \frac{3\epsilon_0}{4\Delta x^2} \sum_{x_n} \left(\hat{a}_{1,x_n} \hat{a}_{1,x_{n-1}} + \hat{a}_{1,x_n} \hat{a}_{1,x_{n+1}} - 2\, \hat{a}_{1,x_n} \hat{a}_{1,x_n} \right) \\
& + \frac{\epsilon_0}{16\Delta x^2} \sum_{x_n} \left(\hat{a}^+_{1,x_{n+1}} \hat{a}^+_{1,x_{n+1}} + \hat{a}^+_{1,x_{n-1}} \hat{a}^+_{1,x_{n-1}} - 2\, \hat{a}^+_{1,x_{n+1}} \hat{a}^+_{1,x_{n-1}} \right) \\
& + \frac{\epsilon_0}{8\Delta x^2} \sum_{x_n} \left(\hat{a}^+_{1,x_{n+1}} \hat{a}_{1,x_{n+1}} + \hat{a}^+_{1,x_{n-1}} \hat{a}_{1,x_{n-1}} - 2\, \hat{a}^+_{1,x_{n-1}} \hat{a}_{1,x_{n+1}} \right) \\
& + \frac{\epsilon_0}{16\Delta x^2} \sum_{x_n} \left(\hat{a}_{1,x_{n+1}} \hat{a}_{1,x_{n+1}} + \hat{a}_{1,x_{n-1}} \hat{a}_{1,x_{n-1}} - 2\, \hat{a}_{1,x_{n+1}} \hat{a}_{1,x_{n-1}} \right) \\
& + \frac{\epsilon_0 c}{4} \sum_{x_n} \left(-\hat{a}_{1,x_n} \hat{a}_{1,x_n} + \hat{a}^+_{1,x_n} \hat{a}_{1,x_n} + \hat{a}_{1,x_n} \hat{a}^+_{1,x_n} - \hat{a}^+_{1,x_n} \hat{a}^+_{1,x_n} \right)
\end{aligned}
$$

Fourier Method Note that some terms of the magnetic field part could be conflated.

$$
\begin{aligned}
H_{pre} = mc^2 & \sum_{\vec{r}_n} \sum_{\lambda} \beta_\lambda \, \hat{c}^+_{\lambda,\vec{r}_n} \, \hat{c}_{\lambda,\vec{r}'_n} \\
& - \mathbf{i}\hbar c \sum_{\vec{r}_n} c^+_{1,\vec{r}_n} \sum_{m=1}^{N_x} D_{x_n,x_m} \, c_{4,x_m y_n z_n} - \mathbf{i}\hbar c \sum_{\vec{r}_n} c^+_{2,\vec{r}_n} \sum_{m=1}^{N_x} D_{x_n,x_m} \, c_{3,x_m y_n z_n} \\
& - \mathbf{i}\hbar c \sum_{\vec{r}_n} c^+_{3,\vec{r}_n} \sum_{m=1}^{N_x} D_{x_n,x_m} \, c_{2,x_m y_n z_n} - \mathbf{i}\hbar c \sum_{\vec{r}_n} c^+_{4,\vec{r}_n} \sum_{m=1}^{N_x} D_{x_n,x_m} \, c_{1,x_m y_n z_n} \\
& - \frac{e}{\sqrt{2}} \sum_{x_n} \left(c^+_{1,x_n} c_{4,x_n} \right) \left(\hat{a}^+_{1,x_n} + \hat{a}_{1,x_n} \right) - \frac{e}{\sqrt{2}} \sum_{x_n} \left(c^+_{2,x_n} c_{3,x_n} \right) \left(\hat{a}^+_{1,x_n} + \hat{a}_{1,x_n} \right) \\
& - \frac{e}{\sqrt{2}} \sum_{x_n} \left(c^+_{3,x_n} c_{2,x_n} \right) \left(\hat{a}^+_{1,x_n} + \hat{a}_{1,x_n} \right) - \frac{e}{\sqrt{2}} \sum_{x_n} \left(c^+_{4,x_n} c_{1,x_n} \right) \left(\hat{a}^+_{1,x_n} + \hat{a}_{1,x_n} \right) \\
& + \frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \left(\sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}^+_{1,x_m y_n z_n} \hat{a}^+_{1,\vec{r}_n} + \sum_{m=1}^{N_x} L_{x_n,x_m} \hat{a}_{1,x_m y_n z_n} \left(\hat{a}^+_{1,\vec{r}_n} + \hat{a}_{1,\vec{r}_n} \right) \right) \\
& - \frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \sum_{m=1}^{N_x} D_{x_n,x_m} \hat{a}^+_{1,x_m y_n z_n} \sum_{m=1}^{N_y} D_{x_n,x_m} \hat{a}^+_{1,x_m y_n z_n} \\
& - \frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \sum_{m=1}^{N_x} D_{x_n,x_m} \hat{a}^+_{1,x_m y_n z_n} \sum_{m=1}^{N_y} D_{x_n,x_m} \hat{a}_{1,x_m y_n z_n} \\
& - \frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \sum_{m=1}^{N_x} D_{x_n,x_m} \hat{a}_{1,x_m y_n z_n} \sum_{m=1}^{N_y} D_{x_n,x_m} \hat{a}^+_{1,x_m y_n z_n} \\
& - \frac{\epsilon_0}{4} \sum_{\vec{r}_n}^{\vec{N}} \sum_{m=1}^{N_x} D_{x_n,x_m} \hat{a}_{1,x_m y_n z_n} \sum_{m=1}^{N_y} D_{x_n,x_m} \hat{a}_{1,x_m y_n z_n} \\
& + \frac{\epsilon_0 c}{4} \sum_{x_n} \left(-\hat{a}_{1,x_n} \hat{a}_{1,x_n} + \hat{a}^+_{1,x_n} \hat{a}_{1,x_n} + \hat{a}_{1,x_n} \hat{a}^+_{1,x_n} - \hat{a}^+_{1,x_n} \hat{a}^+_{1,x_n} \right)
\end{aligned}
$$