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On a Spectral Formulation of Quantum Mechanics

with an Application to Soldering Form of Spin Geometry

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Geometry and Global Analysis

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Except where the reference is made to the work of others, the work presented in the thesis is my own.

Abstract. The main goal of this work is to explore Paschke's *scalar quantum mechanics* (SQM) adequately, in a broad context. In accordance with this goal, we study in an introductory part the motivations leading to SQM. Namely, we notice certain technical difficulties of Bohr's formulation of quantum mechanics and we present Feynman's proof of the Maxwell equation, which directly motivated Paschke's work. Next, we describe language of spectral geometry which is in the formulation of SQM broadly employed. The main part of the thesis deals thoroughly with the central notions of SQM. We show the necessity of the axioms of scalar quantum mechanics and demonstrate their geometric and/or physical meaning. Next, we study nontrivial dynamical systems within the context of the SQM. A system describing the electric Aharonov–Bohm effect, which illustrates the topological obstructions for the existence of a Hamiltonianis, is also presented. After a historical analysis of Dirac's relativistic theory of electron, we deal with a possible extension and an application of the ideas of SQM in the final part. We examine the vacuum given by a complex structure on phase space. which provides a soldering form for internal degrees of freedom furnishing them thus with spatial significance and eventually allowing them to be interpreted as spinors.

Abstrakt. Hlavním cílem předložené disertační práce je studium Paschkeho formulace skalární kvantové mechaniky (SQM) v co nejširším kontextu. Proto je práce rozčleněna na úvodní část, kde studujeme motivace vodoucí k pojmu SQM, zejména technické problémy Bohrovské formulace kvantové mechniky a Feynmanův důkaz Maxwellových rovnic, který byl přímou inspirací k Paschkeho práci. Dále popisujeme zásadní body spektrální geometrie, která je v Paschkeho SQM využita. Hlavní část práce spočívá ve studiu podmínek SQM. Zejména ukazujeme, že Paschkeho podmínky jsou nejen dostačující, ale i nutné, tedy, že žádná nemůže být zeslabena bez důsledků na fyzikální vlastnosti popisovaných systémů. Dále studujeme v rámci SQM netriviální systémy, zejména formulujeme systém popisující elektrický Aharonovův–Bohmův efekt. Tím ilustrujeme topologické překážky existence Hamiltoniánu. V závěrečné části studujeme historii relativistického poisu elektronu a rozšiřujeme myšlenky SQM na relativistivký kontext. Ukzujeme, že vakuum volné kvantové teorie pole, které je popsáno komplexní strukturou na fázovém prostoru, dodává Infeldovy–van der Waerdenovy symboly vnitřních stupňů volnosti a tedy poskytuje popis vztahu vnitřní geometrie ke geometrii prostoru, což umožňuje interpretovat vnitřní stupně volnosti jako spinory.

Introduction

Recently, a new attempt by M. Paschke [32] has appeared to construct quantum theory with minimal assumptions. It has been inspired by Feynman's proof of the Maxwell equations and Paschke calls it *scalar quantum mechanics* (SQM). The main goal of this work is to explore this notion adequately, in a broad context. In accordance with this goal, the thesis is divided into an introductory motivation part, the main part dealing thoroughly with the central notion of SQM and a final part dealing with a possible extension and an application of the ideas of SQM.

The first part of the work (Chapter 1 and 2) is devoted to a careful study of the motivations leading to SQM. In Chapter 1, we recall basic postulates of the orthodox Bohr formulation of quantum mechanics and notice some of its difficulties to draw a comparison to the algebraic formulation of geometric considerations by Paschke.

Next, we recall Feynman's proof of the Maxwell equations, which came to being in 1948 thanks to Feynman's doubts over dogmas of quantum mechanics. After a short review of Feynman's proof in the version reported by F. Dyson in 1990 we study the impact of Feynman's proof in the new paradigm of 1990s, i.e. we study a heritage of Feynman's proof. We put Paschke's work into the context of generalizations of Feynman's proof.

The exposition in Chapter 1 is based on the author's talk [S1] dealing with Bohr formulation and paper [A2], which is a shortened version of the author's talk [C5], dealing with Feynman's proof.

In Chapter 2 we describe language of spectral geometry which is employed in the formulation of SQM. However, in the discussion we also prepare some notions necessary for the application in the final Chapter. The exposition comprises some recent work in progress, which has not been published yet.

In Chapter 3, we address the central notions of Scalar quantum mechanics. We discuss the necessity of the axioms of SQM and clearly demonstrate their geometric and/or physical meaning. We show that reasonable nonrelativistic quantum mechanics is exactly specified by the axioms given by Paschke.

We also treat some nontrivial systems showing the range of applicability of the studied framework. Next, a system describing the electric Aharonov–Bohm effect is presented. It illustrates the topological obstructions for the existence of a Hamiltonian.

The text of this chapter, which is the core of the work, has been published in Journal of Mathematical Physics, see [A3]. A slightly modified and shortened report will appear in [A5]. A preliminary version of the paper was presented at the Workshop on Noncommutative Manifolds in ICTP Trieste [C2] and the 9th International Conference on Squeezed States and Uncertainty Relations Besançon [C3]. Abstract of the latter presentation was published in [A1].

In Chapter 4 we first give a historical account of incipient problems in Dirac's relativistic theory of electron. In this part an extended version of the author's paper [A6] is included. It turns out that difficulties of a relativistic theory are closely related with spin and its soldering form.

Then we turn to the discussion of soldering structures (in a certain context called Infeld–van der Waerden symbols) which have seldom been examined properly. Choosing one of the proposed approaches we show in the final Section that a complex structure on phase space

provides a soldering form for internal degrees of freedom. The exposition of the Section 4.4 has been accepted for publication in Electronic Journal of Theoretical Physics, [A4]. This is a joint work with T. Kopf and A. Lampartová.

To sum it up, the work has a wide scope. In addition to mathematical parts, which are based on clear physical considerations and applications, this work contains thorough remarks on historical background and context of the studied problems. It reflects author's growing passion for history of science.

However, one of the formal problems connected with this thematic breadth is the very different citing style in the aforementioned fields. That is why in the historical parts the references are mainly given in the footnotes (apart from the papers directly used in the mathematical parts of the thesis). In these citations more complete information, e.g., the full name of the journal, the journal number if applicable etc., is provided.

Contents

Chapter 1

Feynman's proof of the Maxwell equations: a quantum mechanics apocrypha

The word apocrypha mostly stands for a biblical text not included the Biblical Canon. Therefore, we first recall the "Biblical Canon of Quantum Mechanic", the unified formulation carried by Niels Bohr, which grew from two different points of view — Heisenberg's matrix mechanics and Schrödinger's wave mechanics — and which have won recognition through the interpretation of Bohr's Copenhagen school. The attention is then drawn to technical difficulties of Bohr's formulation. In the physics expositions they are, in fact, often neglected.

However, there exists yet another formulation of quantum mechanics, different in approach and outlook, but in common situations equivalent. It is the so-called path integral formulation by Richard Feynman. It emanates from Dirac's remarks on the relation of classical action principle to quantum mechanics. Based on the notion of action-at-a-distance, which appeared in Feynman's doctoral thesis (1942), it was fully developed in 1948 ("The Space-Time Formulation of Nonrelativistic Quantum Mechanics").[1]

In the second part of this chapter we dwell upon Feynman's proof of the Maxwell equations. Here we again meet the word apocrypha, this time in its original Greek meaning of that "what was hidden away". Feynman accomplished his proof in early autumn 1948, showed it to Freeman Dyson in October 1948, but he had never published it. This was done as late as in 1990, two years after Feynman's death. We review Dyson's version of the proof and give notice of a new research inspired by Feynman proof. In particular, we explain the role of Feynman proof by the formulation of scalar quantum mechanics.

1.1 Bohr formulation of quantum mechanics

Quantum mechanics as it stands today arose in a short period between 1925 and 1927. This period of time is often called "quantum revolution", since the understanding of physical world had drastically changed.

There is vast amount of literature on the history of quantum mechanics. From the physicists' point of view, there are works by active physicists like, e.g., F. Hund, or mathematician B.L. van der Waerden.[2] For a more historical and less technical account one can consult books by Helge

[1] More details, e.g., in the preface of L.M. Brown (ed.), *Feynman's thesis: a new approach to quantum theory* (World Scientific, Singapore, 2005). Thorough exposition of the path integral formulation can be found in R.P. Feynman and A.R. Hibbs, *Quantum mechanics and path integrals* (McGraw-Hill, New York, 1965).

[2] F. Hund, *Geschichte der Quantentheorie* (BI, Mannheim, 1967). B. L. van der Waerden, *Sources of Quantum Mechanics* (Dover, New York, 1968).

Kragh, Mara Beller and others.[3] A very quick but nice account was given by Brown[4] whereas a huge description elaborated by J. Mehra and H. Rechenberg was strictly criticised.[5]

Let us recall the very basic facts only.

In 1925 **Werner Heisenberg** formulated matrix description of spectroscopy (emission and absorption of light by atoms), which superseded the conception of Niels Bohr. Based on it, foundations of matrix mechanics were laid in a joint work of Max Born and Pascual Jordan ("Zur Quantenmechanik" from autumn 1925) and in the famous 'Dreimännerarbeit' of Born, Heisenberg, and Jordan ("Zur Quantenmechanik II", spring 1926).

In 1926 **Erwin Schrödinger** (in series of four papers "Quantisierung als Eigenwertproblem") introduced his wave mechanics based on a quantum mechanical evolution equation of motion, a differential equation for a wave equation. There are disputes over how much he was influenced by considerations of Louis de Broglie. He also proved (still in 1926) that both approaches to quantum theory, wave and matrix mechanics, are equivalent.[6] The wave functions introduced by Schrödinger provided a first representation of quantum states.

Statistical interpretation of wave function by **Max Born** (from summer 1926) was an important step in formulation of the new probability rules.[7]

Generalization of the Schrödinger wave function and its statistical interpretation were incorporated into matrix mechanics (and the related q-number theory of Paul Dirac) through what came to be known as transformation theory. Independently, Dirac and Jordan developed this new formalism in late 1926 and published it in early 1927.[8] In April 1927 David Hilbert, J. [János, Johann, John] von Neumann and Lothar Nordheim submitted an exposition of Jordan's version of transformation theory;[9] they highlighted some of the mathematical problems in the transformation theory. These problems provided an important stimulus for von Neumann to develop the formalism of Hilbert spaces for quantum mechanics.

Based on quantitative assertions of the latter Dirac work and philosophical views shared with Bohr and Jordan, Heisenberg formulated the uncertainty principle (in more philosophical works sometimes called indeterminacy principle) during his stay in Copenhagen in spring 1927. According to this principle there exist physical quantities, e.g. position and velocity, which cannot be measured simultaneously with an arbitrary precision.[10]

During the autumn 1927, the cornerstone of the interpretation of quantum mechanics had emerged. It was based on indeterminacy principle (W. Heisenberg), complementarity principle

[3]Helge Kragh, *Quantum generations: a history of physics in the twentieth century* (Princeton Univ. Press, Princeton, 1999). M. Beller, *Quantum dialogue: the making of a revolution* (Univ. of Chicago Press, Chicago, 1999).

[4]L M Brown, Quantum mechanics, in: I. Grattan-Guinness (ed.), *Companion encyclopaedia of the history and philosophy of the mathematical sciences* (Routledge, London 1994), 1252–1260.

[5]J. Mehra and H. Rechenberg, *The Historical Development of Quantum Theory*, Vol. I–VI/2 (Springer, New York, Berlin, 1984–2001). Flaws of the first four volumes were pointed out by P. Forman, A Venture in Writing History, *Science* 220 (1983), 824–827.

[6]E. Schrödinger, Über das Verhältnis der Heisenberg–Born–Jordanschen Quantenmechanik zu der meinen, *Annalen der Physik*, IV. Folge, 79 (1926) 734–756; (Volume 384, Issue 8). Cf. also B.L. van der Waerden, From matrix mechanics and wave mechanics to unified quantum mechanics, *Notices AMS* 44 (1997) (3) 323–328.

[7]A. Pais, Max Born's Statistical Interpretation of Quantum Mechanics, *Science* 218 (1982) 1193–1198.

[8]P.A.M. Dirac, The physical interpretation of the quantum dynamics, *Proceedings of the Royal Society of London. Series A, Mathematical and Physical* 113 (1927) 621–641; P. Jordan, Über eine neue Begründung der Quantenmechanik, *Zeitschrift für Physik* 40 (1927) 809–838. The two theories are equivalent, at least formally.

[9]D. Hilbert, J. v. Neumann and L. Nordheim, Über die Grundlagen der Quantenmechanik, *Mathematische Annalen* 98 (1927) 1–30.

[10]W. Heisenberg, Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik, *Zeitschrift für Physik* 43 (1927) 172–198. Historical backgroud is studied in M. Beller, Pascual Jordan's Influence on the Discovery of Heisenberg's Indeterminacy Principle, *Archive for History of Exact Sciences* 33 (1985) 337–349.

(Niels Bohr),[11] correspondence principle (Bohr, Heisenberg and Paul Ehrenfest)[12] and strictly acausal and probabilistic interpretation (Max Born). Formally, it was based on the axiomatic Hilbert space theory (J. von Neumann).

At the Fifth Solvay Conference in October 1927 **Niels Bohr** articulated this interpretation and defended it successfully in tough discussions against the objections raised by the opponents, mainly by Einstein, Schrödinger and de Broglie. However, disputes over the interpretation between Einstein and Bohr lasted more then 20 years.[13] Still, the interpretation gained ascendancy as the correct view of quantum phenomena incredibly quickly.[14] In honour of its Father, the paradigm was called Copenhagen interpretation.

There is a course of *notation* changes neatly connected with the diverse attempts to quantum theory. In the thesis we largely use the so called bra-ket notation invented by **Paul Dirac** in 1938. It is widespread in the physics literature. The name is derived from the use of angle brackets, as Dirac denoted the inner product on a Hilbert space $\mathcal{H}$ by $\langle\varphi \mid \psi\rangle = \langle\varphi| \cdot |\psi\rangle$, with the the right term $|\psi\rangle$ called 'ket' denoting a vector in a Hilbert space $\mathcal{H}$ and the left term $\langle\varphi|$ called 'bra', which is understood as a dual to $|\varphi\rangle$, thus a linear functional on $\mathcal{H}$.

However, Dirac was fond of inventing new notation and terminology. He also originated the use of square brackets $[A, B]$ for Poisson symbols, which was soon taken over to symbolize the quantum mechanical commutator. In 1926 he decided to let the symbol h, commonly used for Planck constant, denote the quantity

$$\frac{h}{2\pi} = 1.054\,571\,628(53) \cdot 10^{-34}\,\mathrm{J\,s}$$

called "Dirac's h" at that time (later rather reduced Planck constant). In 1930 he introduced the symbol $\hbar$ for the reduced Planck constant to avoid misunderstandings. Also the names *bosons* and *fermions* for particles with symmetric (antisymmetric respectively) eigenfunctions stem from Dirac, concretely from one of his lectures in 1945.[15]

1.1.1 Postulates of quantum mechanics

Let us briefly summarize the basic postulates of the Bohr formulation of quantum mechanics. At the same time we provide examples for later reference to the technical difficulties of the formulation in the next section.

(a) State of a physical system is given by normalized vector (equivalence class, more precisely) $|\psi\rangle$ in a separable complex Hilbert space $\mathcal{H}$ with inner product $\langle\phi \mid \psi\rangle$. Two vectors represent the same state if they differ by a phase factor only.

The Hilbert space $\mathcal{H}$ is usually implemented by co called physical Hilbert space $L^2(\mathcal{Q})$ with configuration space $\mathcal{Q}$. For $\mathcal{Q} = \mathbb{R}$, the Hilbert space

$$L^2(\mathbb{R}) = \left\{ f : \mathbb{R} \to \mathbb{C} \;\middle|\; f \text{ measurable } \wedge \int_{\mathbb{R}} |f(x)|^2 \,\mathrm{d}x < \infty \right\},$$

consists of Lebesgue measurable complex-valued functions on $\mathbb{R}$ which are square integrable with respect to the inner product $\langle f \mid g\rangle = \int_{\mathbb{R}} f^*(x) g(x)\,\mathrm{d}x$.

[11] Classical concepts cannot be combined freely in quantum mechanics; this is the source of the so-called wave-particle duality N. Bohr, The quantum postulate and the recent development of atomic theory, *Nature* 121 (1928) 580–590.

[12] Within the limit for large quantum numbers, a quantum description should recover the classical description.

[13] Description of later discussions was given by J. Mehra and H. Rechenberg, *The Historical Development of Quantum Theory*, Vol. VI/2 (Springer, Berlin, 2001), 1197–1208.

[14] J.T. Cushing, *Quantum mechanics: historical contingency and the Copenhagen hegemony* (The Univ. of Chicago Press, Chicago, 1994).

[15] H.S. Kragh, *Dirac – A Scientific Biography* (CUP, Cambridge, 1990), p. 17, 23 and 36.

(b) Time evolution of state of the system can be described by Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle, \tag{1.1}$$

with Hamiltonian operator H.

(c) Measurable quantities, so called physical *observables*, are represented by densely-defined *linear* (i.e. agreeing with the superposition principle) *Hermitian* (i.e. $A = A^\dagger$, in physics literature the same as self-adjoint) operators on $\mathcal{H}$.

(d) Possible values of an observable A in any state belong to the *spectrum* of A. The spectral values of a Hermitian operator are real.

In general spectrum consists of point spectrum, absolute continuous and singular continuous spectra. Below we study some special cases where A has only point spectrum. Then, the possible outcomes of measuring A are given by eigenvalues λ_i of the operator A, i.e., solutions of the eigenvalue equation $A|a_i\rangle = \lambda_i|a_i\rangle$ with the corresponding eigenvectors $|a_i\rangle$.

(e) Measurement probabilities and wave function collapse. For a system in a state $|\psi\rangle = \sum \psi_i|a_i\rangle$, the probability of measuring the value λ_k of the quantity A is equal to $|\langle a_k \mid \psi\rangle|^2$. As $|\langle a_k \mid a_l\rangle|^2 = \delta_{kl}$, we measure out the eigenvalue λ_i with probability 1 for a system in eigenstate $|a_i\rangle$.

The measurement affects the state of the system. If the result of the measurement is λ_k, then the state of the system immediately after the measurement is $|a_k\rangle$. This phenomenon is called wave function collapse.

(f) Correspondence principle. Relations of dynamical variables in classical mechanics and corresponding operators in quantum mechanics differ from each other in the ordering of operators at the most. Classical limit of a quantum system can be obtained, providing the limit exists at all, with large quantum numbers $n \longrightarrow \infty$, which makes Planck constant negligible, $\hbar \longrightarrow 0$.

1.1.2 Technical difficulties of Bohr quantum mechanics

Bohr's formulation of quantum mechanics suffers from some technical difficulties which are only rarely mentioned in elementary physics literature. In rigorous mathematical treatment these difficulties can be improved. Nevertheless, with increasing rigor the theory is getting more complicated. Let us illustrate it on some instructive examples.

Operators, spectra and eigenvectors

For some important operators, e.g. position operator X and momentum operator P, the vectors corresponding to spectral values λ are not normalizable, hence, there do not exist eigenvectors in strict sense.

Let *position operator* X on $\mathcal{H} = L^2(\mathbb{R})$ be defined by

$$X|\psi(x)\rangle = |x\psi(x)\rangle \tag{1.2}$$

on a dense domain $\mathrm{dom}(X) = \{\psi \in L^2(\mathbb{R}) \mid \int_{\mathbb{R}} x^2|\psi(x)|^2\,\mathrm{d}x < \infty\} \subset L^2(\mathbb{R})$.

The eigenvalue equation $X|\psi(x)\rangle = \lambda|\psi(x)\rangle$ gives the spectrum $\sigma(X) = \mathbb{R}$ and functions $\psi_\lambda(x) = \delta(x-\lambda)$ are corresponding eigenvector candidates. However, they are not square integrable, as $\int_{\mathbb{R}} \delta^2(x-x')\mathrm{d}x = \delta(0) \notin \mathbb{R}$. Hence, $\psi_\lambda(x) \notin \mathcal{H}$.

Let *momentum operator* P on $L^2(\mathbb{R})$ be defined by

$$P|\psi(x)\rangle = |-\mathrm{i}\psi'(x)\rangle \tag{1.3}$$

on a dense domain $\mathrm{dom}(P) = \mathcal{C}^1(\mathbb{R}) \cap L^2(\mathbb{R})$. The spectrum $\sigma(P) = \mathbb{R}$ again and the plane waves,

$$\psi_p(x) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}px}\,,$$

which are solutions of the eigenvalue equation, apparently do not belong to $\mathcal{H}$. They do not fulfil necessary condition of square integrability as $\lim_{x\longrightarrow\pm\infty}\psi_p(x)\neq 0$.

We can overcome this difficulty by restricting ourselves to so-called test functions forming a dense subspace in $\mathcal{H}$. It can be taken as the space $\mathcal{C}_c^\infty(\mathbb{R})$ of smooth functions $f:\mathbb{R}\longrightarrow\mathbb{R}$ with compact support. However, in most cases the Schwartz space $\mathcal{S}(\mathbb{R})$ of smooth rapidly decreasing functions on $\mathbb{R}$ is the preferred choice, see [36, Vol. I, Section V.3]. Its advantage is that Fourier transform is in an isometry $\mathcal{S}(\mathbb{R})\longrightarrow\mathcal{S}(\mathbb{R})$. The dual space of $\mathcal{S}(\mathbb{R})$, i.e. the space of tempered distributions $\mathcal{S}'(\mathbb{R})$, contain all the 'interesting' objects, in particular also $\delta(x)$ and $\mathrm{e}^{\mathrm{i}px}$.

Time evolution in quantum mechanics

Let us first note that time is *not* observable in quantum mechanics.

There exist three conceptions of time evolution. In *Schrödinger picture* the state of a system evolves with time and observables do not depend on t. In *Heisenberg picture* time evolution is expressed by time-dependent observables and the state vectors are time-independent. For *Dirac* or *interaction picture* it is specific that both states and observables carry part of the time dependence, however, in a sensibly chosen manner.

In this section we work in Schrödinger picture. Time evolution of a quantum mechanical dynamical system can be described with the help of *time evolution operator* U. If $|\psi,t_0\rangle$ is a state of the system in time t_0, then

$$|\psi,t\rangle = U(t,t_0)|\psi,t_0\rangle.$$

for any later time t. We set $t_0=0$ and denote $U(t)=U(t,0)$. The operator-valued function $U(t)$ is called a *strongly continuous one-parameter unitary group* if it satisfies the following three conditions.

(a) $U(t)$ is a unitary operator: $U^\dagger U=\mathbb{1}$.
(b) $U(t)U(s)=U(t+s)$ for all $t,s\in\mathbb{R}$.
(c) If $t\longrightarrow t_0$, then $U(t)|\psi\rangle = U(t_0)|\psi\rangle$, for all $|\psi\rangle\in\mathcal{H}$. Especially $U(0)=\mathbb{1}$.

Theorem 1.1 (Stone). *Let $U(t)$ be a strongly continuous one-parameter unitary group on a Hilbert space $\mathcal{H}$. Then there is a self-adjoint operator A on $\mathcal{H}$ with $U(t)=\mathrm{e}^{\mathrm{i}tA}$.*

If A is bounded, we can define the exponential by

$$\mathrm{e}^{\mathrm{i}tA}=\sum_{n=0}^{\infty}\frac{(\mathrm{i}t)^nA^n}{n!}.$$

If A is unbounded and self-adjoint, we can define the exponential using functional calculus, cf. [36, Vol. I, Section VIII.3].

If the assumptions of Stone theorem hold, then there exists a generator of time evolution, i.e. Hamiltonian H. It is then obtained by a simple calculation and it reads

$$H=\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0}U(t). \tag{1.4}$$

However, the Hamiltonian H is again an unbounded operator on $\mathcal{H}=L^2(\mathbb{R})$ and we meet the same difficulties in treating the spectral values as above by X,P. Spectrum of H, e.g. for hydrogen atom, consists of several discrete values and a continuous part.

Commutation relations and representations of operators

Again we consider a single particle on $\mathbb{R}$. Commutation relations for position and momentum operators

$$[X,X]=0,\qquad [P,P]=0,\qquad [X,P]=\mathrm{i}\mathbb{1}, \tag{1.5}$$

with $[A, B] := AB - BA$, define fundamental properties of position and momentum operators. Schrödinger representation of X and P, defined in (1.2) and (1.3), is usually used in literature without proving the following hypothesis:

Hypothesis 1.2. *Commutation relations* (1.5) *uniquely determine the representation* (1.2) and (1.3) *of X and P.*

Moreover, as wel shall show, the answer is partial only. The operators X and P are unbounded, hence, only densely defined with $\mathrm{dom}(X), \mathrm{dom}(P) \subsetneq \mathcal{H}$. The same holds for their commutators in (1.5). On the contrary, the right-hand sides of (1.5) are bounded operators. Weyl, who first made an attempt at formulation of the hypothesis,[16] proposed to overcome this difficulty by rewriting the operators into exponential form (it was made precise only later with the help of Stone theorem). Only in this restricted sense, i.e., for the exponential form of (1.5), the answer is positive and it is known under the name Stone–von Neumann theorem (the name was given to it by G. W. Mackey in 1949).

Theorem 1.3 (Stone–von Neumann). *Let $U(r) = \exp(\mathrm{i}Ar)$, $V(s) = \exp(\mathrm{i}Bs)$, $s, r \in \mathbb{R}$, be unitary strongly continuous representations of the group of translations in a Hilbert space $\mathcal{H}$ fulfilling Weyl relations*

$$U(r)V(s) = e^{\mathrm{i}s\cdot r}V(s)U(r). \tag{1.6}$$

Then there exists a decomposition $\mathcal{H} = \bigoplus_{\alpha\in I}\mathcal{H}_\alpha$, where the subspaces $\mathcal{H}_\alpha$ are invariant with respect to $U(r)$, $V(s)$ for all s, r. For every $\alpha \in I$ there exists a unitary operator S_α with

$$(S_\alpha U(r) S_\alpha^{-1}\psi)(x) = \psi(x + r),$$
$$(S_\alpha V(s) S_\alpha^{-1}\psi)(x) = e^{\mathrm{i}s\cdot x}\psi(x).$$

In particular, every irreducible (unitary, strongly continuous) representation of Weyl relations is unitarily equivalent to Schrödinger representation

$$(U(r)\psi)(x) = \psi(x + r), \tag{1.7}$$

$$(V(s)\psi)(x) = e^{\mathrm{i}s\cdot x}\psi(x). \tag{1.8}$$

The idea of the proof was presented by Marshall Harvey Stone (in 1930)[17] and the "strong proof" was completed by John von Neumann.[18]

Remark 1.4. It is easy to show that the representation (1.7), (1.8) is equivalent to the Schrödinger representation (1.2) and (1.3). For the position operator we get

$$(V(s)\psi)(x) = \mathrm{e}^{\mathrm{i}sX}\,\psi(x) = \sum_{k=0}^{\infty}\frac{(\mathrm{i}s)^k X^k}{k!}\psi(x) \overset{(1.2)}{=} \sum_{k=0}^{\infty}\frac{(\mathrm{i}s)^k}{k!}x^k\psi(x) = e^{\mathrm{i}s\cdot x}\psi(x).$$

[16] In the first edition of his book Gruppentheorie und Quantenmechanik from 1928, see [44, §46, p. 207–210].

[17] M. H. Stone, Linear Transformations in Hilbert Space, III. Operational Methods and Group Theory, *Proceedings of the National Academy of Sciences of the USA* **16** (1930)(2) 172–175.

[18] Weyl in the second edition of his *Gruppentheorie und Quantenmechanik* (November 1930) disinguished between "proof" and "strong proof". He also noted that "durchgeführt ist ein solcher Beweis auf anderer Grundlage, wie ich einer brieflichen Mitteilung entnehme, kürzlich von J. v. Neumann" (a footnote to page 248). It was published in J. v. Neumann, Die Eindeutigkeit der Schrödingerschen Operatoren, *Mathematische Annalen* 104 (1931) 570–578. For the history of the Stone–von Neumann theorem see Jonathan M. Rosenberg, A Selective History of the Stone–von Neumann Theorem, in: *Operator algebras, quantization, and noncommutative geometry*, Contemp. Math. **365** (AMS, Providence, 2004) 123–158.

The equivalence for momentum operator is obtained by differentiating (1.7) with respect to the parameter. For the left-hand side we get

$$\frac{\mathrm{d}}{\mathrm{d}r}\bigg|_{r=0} \mathrm{e}^{\mathrm{i}rP}\,\psi(x) = \mathrm{i}P\psi(x) \overset{(1.3)}{=} \frac{\mathrm{d}\,\psi(x)}{\mathrm{d}x},$$

which renders $\mathrm{d}/\mathrm{d}r|_{r=0}\psi(x+r)$, thus providing the desired equivalence.

1.2 Heritage of Feynman's proof

According to Grattan-Guinness,[19] there are two types of writing on the history of mathematics, or more generally history of any science: history and heritage. Both of them are legitimate and important, but it is mostly heritage what is produced by professional mathematicians. However, "the confusion of the two kinds of activity is not legitimate," Grattan-Guinness, p. 165.

By *history* we understand attempts to recount the details of the development of a notion, its origin and the chronology of progress, as far as it can be determined.

The history of Feynman's proof of the Maxwell equation can be told in a brief and simple narrative.[20] In October 1948 it was found out by **Richard P. Feynman**, but remained unpublished. Feynman reported on it only informally to Freeman Dyson and Cécile Morette-de Witt.[21] Only after Feynman's death Dyson disclosed his letters from that time, containing a remark on Feynman's proof.[22] In 1990 Dyson recovered a version of Feynman's proof from his *later* notes and also put Feynman's proof to his view of historical context, see [13].

Heritage, on the other hand, describes the impact of a notion upon later work, especially in the forms which it may take, or be embodied, in later contexts. Some modern form of the studied notion is usually the main focus with attention paid to the course of its development. In the account of heritage mathematical relationships will be noted, but historical ones in the above sense will hold much less interest.

1.2.1 Dyson's version of Feynman's proof

Let us briefly recall Feynman's proof in the form reported by **Freeman J. Dyson**. We have given further details in lecture [C5], see also [A2]. Thorough exposition of Feynman's proof is due to A. Holfter [20].

Theorem 1.5 (Feynman–Dyson). *Let us assume a particle exists with position x_j ($j = 1, 2, 3$) and velocity $\dot{x}_j$ satisfying Newton's equation*

$$m\ddot{x}_j = F_j(x, \dot{x}, t) \tag{1.9}$$

with commutation relations

$$[x_j, x_k] = 0, \tag{1.10}$$

[19] I. Grattan-Guinness, The mathematics of the past: distinguishing its history from our heritage, *Historia Mathematica* 31 (2004) 163–185.

[20] That is why we are concerned with more interesting questions of heritage of Feynman's proof. However, we present our rather historical work later in Section 4.1.

[21] "Feynman had an amazing proof of the Maxwell equations from Quantum Mechanics which I published after his death. He didn't want to publish it, he said it was just a joke," Web of Stories, *Interview of Freeman Dyson by Sam Schweber* from June 1998, Transcript, part 77: Meeting Feynman with Cecil Morette – the proof needed [online, cit. 30. 5. 2010], http://webofstories.com/play/4385. We discuss the reasons why it was not published below.

[22] He read from them for the first time in the talk "Feynman in 1948" at Feynman Memorial Session in 1988. Shortened version of the talk was published in F.J. Dyson, Feynman at Cornell, *Phys. Today* 42 (1989)(2) 32–38. Full text appeared only later in F.J. Dyson, *From Eros to Gaia* (Pantheon Books, New York, 1992), § 34.

(1.11) $$m[x_j, \dot{x}_k] = i\hbar\delta_{jk}.$$

Then there exist fields $E(x,t)$ and $B(x,t)$ satisfying the Lorentz force equation

(1.12) $$F_j = E_j + \epsilon_{jkl}\dot{x}_k B_l$$

and the Maxwell equations

(1.13) $$\nabla \cdot B = 0,$$

(1.14) $$\frac{\partial B}{\partial t} + \nabla \times E = 0.$$

Remark: The other two Maxwell equations

(1.15) $$\nabla \cdot E = 4\pi\rho,$$

(1.16) $$\frac{\partial E}{\partial t} - \nabla \times B = 4\pi j,$$

merely define the external charge and current densities ρ and j.

Dyson's version of the proof [13] was repeated and commented many times in the literature. We refer to thorough treatment by Holfter [20] stressing the geometry hidden in the original and by Cariñena & al. [4] formulated in the language of Poisson geometry.

Before sketching the proof let us make some brief comments. The essential idea seems to be using velocity $\dot{x}_i$ instead of momentum p_i in the commutation relation (1.11), which renders the dynamics better. Also, key ingredients of the proof are properties of the commutator, namely

(i) Jacobi identity (expressing associativity)

(1.17) $$[A,[B,C]] + [C,[A,B]] + [B,[C,A]] = 0,$$

(ii) Leibniz rule (giving the structure of derivatives)

(1.18) $$[A, BC] = [A,B]C + B[A,C],$$

(1.19) $$\frac{\mathrm{d}}{\mathrm{d}t}[A,B] = \left[\frac{\mathrm{d}A}{\mathrm{d}t}, B\right] + \left[A, \frac{\mathrm{d}B}{\mathrm{d}t}\right].$$

Sketch of the proof. Total time derivative of (1.11), using (1.19) and (1.9) gives $m[\dot{x}_j, \dot{x}_k] + [x_j, F_k] = 0$. Hence, $[x_i, F_j]$ is antisymmetric with respect to swapping the indices. In the next step, regarding Jacobi identity, we get $[x_k, [x_i, F_j]] = 0$ and $[x_i, F_j]$ depends on x and t only. Thus, $[x_i, F_j] = -(i\hbar/m)\epsilon_{ijk}B_k$ and we can define

(1.20) $$B_l = \frac{m^2}{2i\hbar}\epsilon_{lkm}[\dot{x}_k, \dot{x}_m].$$

Equation (1.13) follows by another application of Jacobi identity.

Next Lorentz force equation (1.12) is taken into account. It is satisfied by assuming it to be definition of electric field E. Similarly as above for B it is shown that $E = E(x,t)$.

Faraday law (1.14) is proved by total time derivative of (1.20) using (1.12) in the Newton's law (1.9). □

However, to understand properly the history of Feynman's proof, one has to see it in its historical context, i.e., in the context of the development of Feynman's ideas on quantum physics. In summer 1948 Feynman tried hard to 'crack the riddle' of Quantum electrodynamics (QED). For him the proof of Maxwell equations was confirmation of the basic dogmas of quantum mechanics. He made sure for himself that the renormalization problem in QED can not be solved by introducing more general particle theory outside the standard framework. As noted by Dyson, the proof told him that there are no models that could not be described by an ordinary Lagrangian or Hamiltonian. From Feynman's point of view the proof was a failure, not a success. Therefore, he was not interested in publishing it.

1.2.2 Feynman's proof in a new paradigm

"It is not only a historical relic of a failed program. It also raises some new questions."

F. Dyson, [13, p. 211]

After the publication of Feynman's proof with Dyson's editorial comment in 1990, see [13], it was not considered to be just a historical feature, it inspired immediately new research directions. We review the discussion about symmetries in Feynman's proof and then we discuss relation with the inverse problem of the calculus of variations first pointed out by Hojman and Shepley. Generalizations of Feynman's proof to arbitrary (even noncommutative) configuration spaces are also mentioned. They are then discussed more thoroughly in the next Chapter, as they led to the notion of scalar quantum mechanics, the central notion of this thesis. Finally, we also mention some attempts to introduce new particle dynamics into Feynman's proof. We shall discuss including of the internal degrees of freedom into Feynman's proof in Section 1.2.3. However, it is closely connected with extension of Feynman's problem on internal degrees of freedom. Namely, the internal space usually renders the configuration space noncommutative.

Dyson emphasized a question concerning a then fashionable theory of symmetries. The Maxwell equations are relativistically invariant, while Newtonian assumptions (1.9)–(1.11) are nonrelativistic. "The proof begins with assumptions invariant under Galilean transformations and ends with equations invariant under Lorentz transformations. How could this have happened?"

Immediate comments focused mainly on this question.[23] It was stressed that the answer lies in the nonhomogeneous Maxwell equations (1.15), (1.16), which were taken just to define sources ρ and j. They are of course not Galilean invariant. Dombey pointed out that an earlier definition by Levy-Leblond

$$\nabla \cdot E = 4\pi\rho, \qquad \nabla \times B = 4\pi j,$$

keeps Galilean invariance. However, in this so-called magnetic limit one must give up magnetic forces between electric currents. The other authors solved the issue by asserting that *full* set of Maxwell equations can not be derived from Galilean transformation.

Feynman's proof and the inverse problem of the calculus of variations

S.A. Hojman and L.C. Shepley considered Feynman's proof in the context of the inverse problem of the calculus of variations. From this point of view, Feynman's proof tells us that we can quantize only such equations (1.9), which are describable in the form of Euler–Lagrange equations with Lagrangian L of electromagnetic form.

Hojman and Shepley were looking for a variational integrating factor (variational multiplier), i.e a nonsingular symmetric matrix w_{ij} with elements depending on t, x and $\dot{x}$, and a function $L(t, x, \dot{x})$ such that

$$w_{ij}(\ddot{x}^j - f^j) = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}^i} - \frac{\partial L}{\partial x^i}.$$

The necessary and sufficient condition for the existence of a Lagrangian L are the well-known Helmholtz conditions of the (weak) inverse problem of the calculus of variations.[24] If L exists, then the variational integrating factor is given by

$$w_{ij} = \frac{\partial^2 L}{\partial \dot{x}^i \partial \dot{x}^j}.$$

[23] Four independent comments, by N. Dombey, R.W. Brehme, J.L. Anderson and I. E. Farquhar, appeared in *American Journal of Physics* 59 (1991)(1) 85–87. Further, it was commented by A. Vaidya and C. Farina, Can Galilean mechanics and full Maxwell equations coexist peacefully? *Physics Letters A* 153 (1991)(6–7) 265–267; and H.P. Noyes, Preprint SLAC-PUB-5588 (November 1991).

[24] More precisely Helmholtz conditions for integrating factor. See, e.g., O. Krupková, *The Geometry of Ordinary Variational Equations*, Lecture Notes in Mathematics 1678 (Springer, Berlin, 1997).

They generalized Feynman's assumption (1.11), assuming

$$[X^i, \dot{X}^j] = \mathrm{i}\hbar G^{ij}, \tag{1.21}$$

with capital letters denoting quantum mechanical operators, where the commutators form a symmetric array, $G^{ij} = G^{ji}$. They proved that matrix inverse of the classical analogue of G^{ij} became w_{ij}, satisfying Helmholtz conditions, hence, giving a Lagrangian. The existence of a Lagrangian essentially comes from (1.10). The explicit form of L is determined by (1.21). In accordance with the well-known fact L is determined up to an overall multiplicative constant and an addition of a total time derivative.

In further comments Hughes used variational multipliers of the trivial form $w_{ij} = \delta_{ij}$,[25] i.e., such that employ only strong variationality conditions.[26] Variational multipliers of slightly more general form $w_{ij} = \mathrm{e}^{\lambda t}\,\delta_{ij}, \lambda \in \mathbb{R}$ were used in a comment by Moreira.[27]

Later, J.F. Cariñena, L.A. Ibort, G. Marmo and A. Stern used the inverse problem of the calculus of variations in the study of Lagrangian realizations of Poisson brackets defining a particle with internal degrees of freedom, see [4, Section 8].

Feynman's proof on arbitrary configuration spaces

Using Poisson geometry **J.F. Cariñena, L.A. Ibort, G. Marmo** and **A. Stern** generalized Feynman's proof to arbitrary configuration spaces of classical mechanics, see [4, Section 5–7].

Analysing hidden assumptions of Feynman's proof, **M. Paschke** achieved a generalization of the original quantum-mechanical Feynman's proof to arbitrary configuration spaces, avoiding a choice of local coordinates at the same time, see [32]. He came to the notion of scalar non-relativistic quantum mechanics, which is studied thoroughly in the next Chapter.

Feynman's proof was also generalized for some noncommutative configuration spaces. In 2003 two independent papers appeared, where the authors considered Feynman's proof on Moyal deformed $\mathbb{R}^n$.

A. Boulahoual and **M. B. Sedra**[28] studied two types of noncommutativity on Moyal deformed $\mathbb{R}^3$. First they assume

$$[x_j, x_k]_* = \mathrm{i}\theta_{jk}, \qquad \text{with} \qquad \theta_{jk} \in \mathbb{C}, \tag{1.22}$$

where $[\cdot\,,\cdot]_*$ is a so-called Moyal bracket defined by $*$-product. They claim that fields E, B in the Lorentz force have no spatial dependence, hence, this form of noncommutativity induces static Maxwell equations, cancelling the charge and current densities.

The second type of noncommutativity consists in the assumption

$$m[x_j, \dot{x}_k] = \delta_{jk} + \mathrm{i}m\theta_{jk} f(x,t) \tag{1.23}$$

in addition to the first type. They claim to derive a nontrivial noncommutative extension of the homogeneous Maxwell equations.

However, it was later shown by J.F. Cariñena and H. Figueroa in [5] that their conclusions are not correct.

[25] R.J. Hughes, On the Feynman's proof of the Maxwell equations, *American Journal of Physics* 60 (1992)(4) 301–306.

[26] However, his historical comments to the inverse problem are inaccurate. Cf. my paper J. Kotůlek, Z historie inverzního variačního problému: Odvození podmínek silné variačnosti, *Pokroky matematiky, fyziky a astronomie* 48 (2003)(3) 222–238.

[27] Ildeu de Castro Moreira, Comment on "On the Feynman's proof of the Maxwell equations" by R.J. Hughes, *American Journal of Physics* 61 (1993)(9) 853.

[28] Noncommutative geometry framework and the Feynman's proof of Maxwell equations, *Journal of Mathematical Physics* 44 (2003)(12), 5888–5901.

A. Holfter [20] discussed Moyal deformed $\mathbb{R}^n$, i.e. he took

$$[x_j, x_k] = \mathrm{i}\theta_{jk}, \qquad \theta_{jk} \in \mathbb{C}, \qquad j,k = 1,\dots,n, \tag{1.24}$$

instead of (1.10), providing noncommutativity of local coordinates. He was able to deduce that the external force F is linear in velocities and he got some properties of E and B fields, but did not derive the Maxwell equations.

Then, in [20, Section 6.8], he considered a noncommutative configuration space given by the algebra $\mathcal{A} = \mathcal{C}^\infty(\mathbb{R}^m) \otimes M_n(\mathbb{C})$, which can be used to describe spinning particle on $\mathbb{R}^3$.

J.F. Cariñena and H. Figueroa in [5] follow up using Poisson geometry developed in [4]. They drop locality assumption for a classical particle on configuration manifold $\mathcal{Q}$ by setting

$$\{x^i, x^j\} = g_{ij}(x) \tag{1.25}$$

with g_{ij} an antisymmetric matrix such that the Poisson bracket $\{\,\cdot\,,\cdot\,\}$ fulfils Leibniz rule (1.18). With the help of Jacobi identity they show that g_{ij} must be constant. (The dependence of g on $\dot{\boldsymbol{x}}$'s is studied later in their paper.)

They derived a generalization of the first Maxwell equation (1.13)

$$\nabla B = -\frac{1}{m} B \cdot \dot{\nabla} \times B, \tag{1.26}$$

which reduces to (1.13) if field B is independent of $\dot{\boldsymbol{x}}$'s. Similarly, their resulting second Maxwell equation

$$(\nabla \times E)_k = -\frac{\partial B}{\partial t} + \frac{1}{m}\left((\dot{\nabla} \cdot E) B_k - (E \cdot \dot{\nabla}) B_k - B \cdot \frac{\partial E}{\partial \dot{\boldsymbol{x}}^k} \right) \tag{1.27}$$

reduces to (1.14) if fields B, E are independent of $\dot{\boldsymbol{x}}$'s. So, in the limit, they obtained a smooth transition into the commutative case, contrary to what is claimed by Boulahoual and Sedra.

Finally, they consider $g_{ij}(x, \dot{\boldsymbol{x}})$ and generalize simultaneously also (1.11) to

$$m\{x^i, \dot{\boldsymbol{x}}^j\} = \delta_{ij} + f_{ij}(x, \dot{\boldsymbol{x}}), \tag{1.28}$$

with f_{ij} another antisymmetric matrix compatible with the Poisson bracket properties. They claim to derive "equations a bit more involved, but similar" to (1.26) and (1.27). Nevertheless, the corresponding formulae are not stated.

Continuing their previous work from 2003, **M. Paschke** and **T. Kopf** [25] generalized the notion of scalar quantum mechanics to some noncommutative configuration spaces, again in coordinate-free manner. This work, published only in 2007, provided algebraic version of Feynman's proof on noncommutative spaces.

They studied several important models, e.g. the algebra $\mathcal{A} = \mathcal{C}^\infty(\mathcal{Q}) \otimes M_n(\mathbb{C})$ which leads to non-Abelian Yang–Mills theories, the two-point model with $\mathcal{A} = \mathcal{C}^\infty(\mathcal{Q}) \otimes (\mathbb{C} \oplus \mathbb{C})$ or noncommutative tori $\mathbb{T}^n_\theta$. They examined models over Moyal-deformed plane $\mathbb{R}^2_\theta$ with results in accordance with those of J.F. Cariñena and H. Figueroa [5].

1.2.3 Including internal degrees of freedom

We finish this chapter by a few short remarks on Feynman's proof with internal degrees of freedom. Namely, our work presented in Section 4.4, i.e., a derivation of spin soldering from rather general physical considerations, can be understood as a form of Feynman's proof for spinning particles, thus particles with internal degrees of freedom "soldered" to the spacetime geometry.

In August 1990 a paper by **C.R. Lee** [28] appeared where the motion of a particle with isospin under the influence of non-Abelian gauge field is studied and homogeneous Yang–Mills

equations are obtained. However, Farquhar criticized the approach,[29] as it does not furnish the (non-homogeneous) equations with necessary transformation properties. The same critique refers also to the original Dyson version of Feynman's proof.[30] A special relativistic version of the arguments by Lee was published by Tanimura, [38].

However, the isospin is an example of internal degree of freedom which does not possess soldering structures.

Shogo Tanimura was the first to ask if we can involve spin in the arguments of Feynman's proof, see [38, p. 247]. He remarks that he "naively expects that the Lie algebra of the local Lorentz group

$$[S_{\mu\nu}, S_{\rho\sigma}] = -\mathrm{i}\,\hbar(g_{\mu\rho}S_{\nu\sigma} - g_{\nu\rho}S_{\mu\sigma} - g_{\mu\sigma}S_{\nu\rho} + g_{\nu\sigma}S_{\mu\rho})$$

leads to the equation for force which electromagnetic and gravitational fields exert over a particle with spin" according to van Holten:[31]

$$m\ddot{\mu} = eg^{\mu\nu}F_{\nu\rho}\dot{x}^{\rho} - m\Gamma^{\mu}{}_{\nu\rho}\dot{x}^{\nu}\dot{x}^{\rho} + \frac{e}{2m}g^{\mu\nu}(\nabla_{\nu}F_{\rho\sigma})S^{\rho\sigma} + \frac{1}{2}R^{\mu}{}_{\nu\rho\sigma}\dot{x}^{\nu}S^{\rho\sigma},$$

where e is electric charge of the particle, which has been absorbed in the definition of $F_{\mu\nu}$ in the previous sections; ∇ denotes covariant derivative with the Levi-Civita connection $\Gamma^{\mu}{}_{\nu\rho}$; $R^{\mu}{}_{\nu\rho\sigma}$ is the Riemann curvature tensor and $S^{\rho\sigma}$ is intrinsic angular momentum tensor, that is, spin. The derivation is, however, "left for a future work".

Chihong Chou generalized Feynman's proof to spinning particles on a flat (2+1)-dimensional spacetime in [6]. He assumed, in addition to Feynman's assumptions, the existence of Hamiltonian evolution, in order to utilize the framework of symplectic geometry, cf. [38, p. 233]. Moreover, he did not consider deriving anything like soldering form.

Thorough exposition of Feynman's proof with internal degrees of freedom by **J.F. Cariñena, L.A. Ibort, G. Marmo and A. Stern** appeared in 1995, see [4].[32]

[29] Comment in *Physics Letters A* 151 (1990)(5) 203–204.

[30] See also footnote 23.

[31] J.W. van Holten, On the electrodynamics of spinning particles, *Nuclear Physics B* 356 (1991)(1), 3–26.

[32] However, a part of the exposition is based on an earlier paper of one of the authors, namely A. Stern and I. Yakushin, Deformed Wong particles, *Physical Review D* 48 (1993)(10) 4974–4979.

Chapter 2

Notion of spectral triple

In spectral geometry, the space is usually described by the notion of *spectral triple* $(D, \mathcal{A}, \mathcal{H})$. It consists of a distinguished unbounded self-adjoint operator D (e.g., Dirac or Laplace operator, depending on situation) and an algebra $\mathcal{A}$, both (faithfully) represented on a Hilbert space $\mathcal{H}$. However, the concrete spectral triples may differ slightly in details. For example, we should add some other structures for D to play the role of Dirac operator $\not{D}$ (operators specifying the spin structure, etc.). Note that we do not restrict the order of D from the beginning.

Although we are going to modify some attributes of the spectral triples, let us recall the features which we build upon. First, the operator D allows us to define a concept of smoothness and we can require the algebra to meet its criteria.

2.1 Smoothness in spectral geometry

Motivated by physics, the operator D is often explicitly chosen to be a differential operator. Its commutator with a coordinate operator results in a differential expression. Hence, the existence of this differential expression (or its properties) refers to some requirements for smoothness of the coordinate.

Let us begin with some illustrative examples. We choose $\mathcal{A} = \mathcal{C}^\infty(S^1)$, the commutative algebra of complex-valued functions on a circle, and Hilbert space $\mathcal{H} = L^2(S^1, S^1 \times \mathbb{C})$ consisting of square integrable sections of the complex line bundle $\pi : S^1 \times \mathbb{C} \longrightarrow S^1$, cf. Section 3.2 below.

Example 2.1. Let $D = -\mathrm{i}(\partial/\partial\varphi)$ be differential operator of the first order. This can be expressed by

$$[D, a] \in \mathcal{A} \qquad \forall a \in \mathcal{A},$$

whereas $[D, a] = -\mathrm{i}(\partial a(\varphi)/\partial\varphi)$ by Lemma 3.3, equation (3.5b), below. Equivalently, we can write it in the following form

$$[[D, a], b] = 0 \qquad \forall a, b \in \mathcal{A}.$$

The fact that $a \in \mathcal{A}$ possesses derivative of the n-th order implies that the operator

$$[\underbrace{D, [D, [D, \dots [D}_{n \text{ times}}, a] \cdots]]] = (-\mathrm{i})^n \frac{\partial^n a(\varphi)}{\partial\varphi^n}$$

is bounded.

Example 2.2. Let $D = -\partial^2/\partial\varphi^2$ be Laplace operator. As the operator is of the second order, the corresponding condition reads as

$$[[D, a], b] \in \mathcal{A} \qquad \forall a, b \in \mathcal{A},$$

or, equivalently by $[[[D,a],b],c]=0$ for all $a,b,c\in\mathcal{A}$.

The equality

$$[D,a]=-\frac{\partial^2 a(\varphi)}{\partial\varphi^2}-2\frac{\partial a(\varphi)}{\partial\varphi}\frac{\partial}{\partial\varphi},$$

cf. Lemma 3.3, equation (3.5c) below, defines a differential operator of the first order containing first two derivatives of $a(\varphi)$. Hence, the existence of $[D,a]$ ensures the existence of the first two derivatives of $a(\varphi)$.

In these examples, where D is a differential operator, the smoothness reflects the existence of derivatives. However, based on a spectral decomposition of D, our notion of smoothness will be more abstract.

Let us recall that *spectrum* $\sigma(D)$ of the operator D is a set of complex numbers λ such that the mapping $D-\lambda\mathbb{1}:\mathrm{dom}(D)\longrightarrow\mathcal{H}$ is not a bijection. A subset of eigenvalues $\lambda\in\sigma(D)$ with corresponding eigenvectors $\psi_\lambda\in\mathcal{H}$ satisfying the equation

$$D|\psi_\lambda\rangle=\lambda|\psi_\lambda\rangle$$

is called *point spectrum*. For the values $\lambda\in\sigma(D)$ not contained in point spectrum, the operator $D-\lambda\mathbb{1}$ is not continuously invertible and there exist only generalized corresponding eigenvectors, for an example see Section 1.1.2.

Example 2.1. (continued) As the spectrum of $D=-\mathrm{i}(\partial/\partial\varphi)$ contains only discrete eigenvalues, the situation is particularly simple. The eigenvalue equation

$$-\mathrm{i}\,\frac{\partial}{\partial\varphi}\psi_\lambda(\varphi)=\lambda\psi_\lambda(\varphi)$$

is easily solved by separation of variables, $\psi_\lambda(\varphi)=\psi_0\mathrm{e}^{\mathrm{i}\,\lambda\varphi}$, $\psi_0\in\mathbb{C},\lambda\in\mathbb{R}$. Employing the boundary condition $\psi_\lambda(0)=\psi_\lambda(2\pi)$, i.e. $\mathrm{e}^{\mathrm{i}\,\lambda 0}=\mathrm{e}^{2\pi\mathrm{i}\,\lambda}$ we get $\lambda\in\mathbb{Z}$. Hence, $\sigma(D)=\mathbb{Z}$ with corresponding 1-dimensional eigenspaces $\mathbb{C}\cdot\mathrm{e}^{\mathrm{i}\,\varphi n}$.

Example 2.2. (continued) The spectrum of $D=-\partial^2/\partial\varphi^2$ is once again purely discrete. The eigenvalue equation

$$-\frac{\partial^2}{\partial\varphi^2}\psi_\lambda(\varphi)=\lambda\psi_\lambda(\varphi)$$

is solved by

$$\psi_\lambda(\varphi)=C_1\mathrm{e}^{\mathrm{i}\,\sqrt{\lambda}\varphi}+C_2\mathrm{e}^{-\mathrm{i}\,\sqrt{\lambda}\varphi},\qquad C_1,C_2\in\mathbb{C}.$$

Employing boundary conditions

$$\psi_\lambda(0)=\psi_\lambda(2\pi),\qquad \left.\frac{\partial}{\partial\varphi}\right|_{\varphi=0}\psi_\lambda(\varphi)=\left.\frac{\partial}{\partial\varphi}\right|_{\varphi=2\pi}\psi_\lambda(\varphi),$$

we get $\sqrt{\lambda}\in\mathbb{Z}$, hence, $\sigma(D)=\{0,1^2,2^2,3^2,\ldots\}=\{0,1,4,9,\ldots\}$,[1] with 1-dimensional eigenspace $\mathbb{C}\cdot\mathbb{1}$ corresponding to the eigenvalue $n=0$ and with 2-dimensional eigenspaces $\mathbb{C}\cdot\mathrm{e}^{\mathrm{i}\,\varphi n}+\mathbb{C}\cdot\mathrm{e}^{-\mathrm{i}\,\varphi n}$ corresponding to all other eigenvalues $n\neq 0$.

[1] From the physical point of view it is the energy spectrum of a free particle on a circle, in the system of units set by $\hbar=m=1$.

A point spectrum with finite-dimensional eigenspaces is a typical result for Dirac and Laplace operators on compact manifolds. We have devoted our study to this situation, which is both interesting and nontrivial, as we believe. However, the case of noncompact manifold, which is not treated in the thesis, is important as well. We have already noticed some inconveniences related to this more complicated situation in Section 1.1.2.

Our eigenvectors from the examples above are smooth functions from $\mathcal{H} = L^2(S^1, S^1 \times \mathbb{C})$. Nevertheless, $\mathcal{H}$ contains many functions that are not differentiable and are, therefore, not contained in the domain of either the unbounded operator D or its power D^n for any $n \in \mathbb{N}$. It enables us to define the smoothness with respect to D as a notion on the Hilbert space $\mathcal{H}$. For this we shall now study the reasons why there are some vectors not contained in the domain of D.

First, let us number the eigenvalues of D. We take $\{(\lambda, \psi_\lambda)\}$, a set of couples with a discrete eigenvalue $\lambda \in \sigma(D)$ and a corresponding eigenvector ψ_λ. If the eigenspace corresponding to λ has dimension m, then there are m couples with the first term λ in the set. Next, we number the elements of $\{(\lambda, \psi_\lambda)\}$ with integers by $|\lambda|$, say $n \longrightarrow (\lambda, \psi_\lambda)_n$, where the order of the couples with $|\lambda_i| = |\lambda_j|$ does not matter. It induces a numbering $n \longrightarrow \lambda_n$ of the eigenvalues λ of D.

If D has purely point spectrum, as we assume, then there exists a basis of $\mathcal{H}$ consisting merely of eigenvectors of D. Any $v \in \mathcal{H}$ can be decomposed into components from the eigenspaces of D:

$$v = \sum_{\lambda \in \sigma(D)} v_\lambda.$$

In this form we can easily describe how D acts on v. If the result exists, it is given by

$$Dv = \sum_{\lambda \in \sigma(D)} Dv_\lambda = \sum_{\lambda \in \sigma(D)} \lambda v_\lambda.$$

The sum on the right-hand side is finite if

$$\Big\| \sum_{\lambda \in \sigma(D)} \lambda v_\lambda \Big\|^2 = \sum_{\lambda, \mu \in \sigma(D)} \langle \lambda v_\lambda \mid \mu v_\mu \rangle = \sum_{\lambda \in \sigma(D)} |\lambda|^2 \|v_\lambda\|^2 < \infty, \tag{2.1}$$

where we used $\langle v_\lambda \mid v_\mu \rangle = 0$ for $\lambda \neq \mu$. The condition (2.1) on v is nontrivial, as $|\lambda| \longrightarrow \infty$. If we require $\|D^n v\|^2 < \infty$, it is getting even more strict with increasing n:

$$\sum_{\lambda \in \sigma(D)} |\lambda|^{2n} \|v_\lambda\|^2 < \infty. \tag{2.2}$$

We see that v is smooth only if its components in eigenspaces corresponding to high eigenvalues decrease sufficiently quickly. Particularly, we can take the smooth vectors from the following subspaces:

$$\mathcal{H}^{\text{fin}} = \{v \in \mathcal{H} \mid v_\lambda \neq 0 \text{ for only finite number of } \lambda \in \sigma(D)\},$$
$$\mathcal{H}^\infty = \Big\{ v \in \mathcal{H} \,\Big|\, \sum_{\lambda \in \sigma(D)} |\lambda|^{2n} \|v_\lambda\|^2 < \infty \, \forall n \in \mathbb{N} \Big\}.$$

A bounded operator $T : \mathcal{H} \longrightarrow \mathcal{H}$ is called *smooth* (with respect to D) if it preserves smooth vectors from $\mathcal{H}^\infty \subset \mathcal{H}$. More precisely, we require its restriction to $\mathcal{H}^\infty$ to be a mapping $T|_{\mathcal{H}^\infty} : \mathcal{H}^\infty \longrightarrow \mathcal{H}^\infty$.

Example 2.3. Consider D with $\sigma(D) = \mathbb{N}$ and 1-dimensional eigenspaces $\mathcal{H}_n$, $n \in \mathbb{N}$, Hilbert space $\mathcal{H} = \bigoplus_{n \in \mathbb{N}} \mathcal{H}_n$ with basis formed by eigenvectors $|\varphi_n\rangle \in \mathcal{H}_n$, $\|\varphi_n\| = 1$ and operator $T : \mathcal{H} \longrightarrow \mathcal{H}$ given by

$$T|\varphi_n\rangle = |\varphi_{2^n}\rangle \tag{2.3}$$

The operator T is clearly bounded. Indeed, for $|x\rangle = \sum_n x^n|\varphi_n\rangle \in \mathcal{H}$ we get

$$\|Tx\|^2 = \Big\langle T\sum_n x^n\varphi_n \,\Big|\, T\sum_m x^m\varphi_m\Big\rangle = \sum_{m,n}(x^*)^n x^m\langle T\varphi_n \mid T\varphi_m\rangle =$$

$$= \sum_{m,n}(x^*)^n x^m \underbrace{\langle\varphi_{2^n} \mid \varphi_{2^m}\rangle}_{\delta_{mn}} = \sum_n |x^n|^2 = \|x\|^2.$$

Hence,

$$\|T\| = \sup\frac{\|T|x\rangle\|}{\||x\rangle\|} = 1.$$

Take a vector $|v\rangle = \sum_n 2^{-n/2}|\varphi_n\rangle$. As $\|D^k|v\rangle\|^2 = \sum_n n^{2k}2^{-n}$ is convergent, the vector $|v\rangle$ is smooth. However, $\|D^k|Tv\rangle\|^2 = \sum_n (2^n)^{2k}2^{-n}$ is divergent for $k \geq 1$ and T is not smooth.

Intuitive explanation for this is that T maps eigenvectors with small eigenvalues with respect to D onto vectors with high eigenvalues. It differs widely from a diagonal operator to D.

We note that, if T is smooth with respect to D, then $[D, T]$ is bounded.

If we restricted ourselves to a subspace

$$\mathcal{H}_K = \bigoplus_{\substack{\lambda\in\sigma(D)\\ |\lambda|\leq K}} \mathcal{H}_\lambda, \tag{2.4}$$

where the operator D is bounded, $\|D|_{\mathcal{H}_K}\| = K$, all problems with D would disappear. Nevertheless, every attempt on establishing locality leads to violation of $\mathcal{H}_K$.

2.2 Spectral construction of $\mathcal{A}$

Having discussed operator D, we should add an algebra $\mathcal{A}$ now. However, it seem to be a very strong restriction to require $\mathcal{A}$ to contain only operators smooth with respect to D. Connes was trying for a long time to do without it or to replace it by something else, but the operator D alone does not specify the geometry. However, this is core of the problem of hearing the shape of a drum.[2]

We specify the algebra indirectly by introducing some structures on spectral decomposition of $\mathcal{H}$ with respect to D. This information on D allows us to reconstruct coordinates, which are automatically smooth. Nevertheless, this procedure preserves some freedom of choice. Restrictions imposed by the procedure on spectral geometry remain to be studied.

Intuitively, we understand D being fundamental multi-dimensional or perhaps no-dimensional object. Introducing the dimension means regular numbering of the eigenspaces of D. The numbering function is called *transporter* p and we require that its spectrum is formed by regular numbers, that it has isomorphic eigenspaces and that it is in accordance with D in the following sense: D and p have common eigenspaces and there is a sensible relation of the corresponding numberings. Let us state it more precisely.

Definition 2.4. An unbounded self-adjoint operator p is called *transporter with respect to* D if the following conditions are satisfied:

(a) $\sigma(p) = \mathbb{Z}$.

(b) $P_\lambda \sim P_\mu$ for $\lambda, \mu \in \sigma(p)$. More precisely, projectors P_λ on the eigenspaces corresponding to λ are related by unitary transformations: $P_\lambda = U^{-1}P_\mu U$.

[2]The problem was posed by Mark Kac in the famous paper "Can one hear the shape of a drum?" See *American Mathematical Monthly* **73** (1966)(No. 4, part 2) 1–23. In two dimensions it remained open until 1992, when it was solved by Gordon, Webb, and Wolpert. The answer is that we can deduce some information, but for many shapes we cannot hear the shape *completely*.

(c) $[p, D] = 0$.
(d) Let $\Lambda(n) = \{\lambda \mid \exists|\psi\rangle : D|\psi\rangle = \lambda|\psi\rangle \wedge p|\psi\rangle = n|\psi\rangle\}$. There exist $C, k, N \in \mathbb{N}$ such that for all $n \in \mathbb{Z}$ with $n > N$ it holds

$$\sup \frac{\Lambda(n+1)}{\Lambda(n)} < C \cdot \lambda^{2k} \qquad \forall \lambda \in \Lambda(n).$$

Remark 2.5. (i) The definition might be adjusted according to the interesting cases under consideration, e.g. to guarantee the properties only asymptotically, for high eigenvalues of p and D.

(ii) As n-dimensional geometry admits more than one transporter, it is necessary to clarify their relation. We work here with the commuting set of transporters only, i.e. $\{p_i\}$ with $[p_i, p_j] = 0$ for all i, j.

Relations among the eigenspaces of transporter p are governed by rising operator u:

Definition 2.6. Unitary operator u is called *rising operator of transporter* p if

$$[p, u] = u. \tag{2.5}$$

Proposition 2.7. *Contraction of operator u on the eigenspace of p corresponding to eigenvalue n,*

$$u|_{\mathcal{H}_n} : \mathcal{H}_n \longrightarrow \mathcal{H}_{n+1}$$

is an isometry.

Proof. The operator u is unitary, hence isometry. Contraction of isometry is isometry. It remains to show that for $v \in \mathcal{H}_n$ is $uv \in \mathcal{H}_{n+1}$:

$$p|uv\rangle \overset{(2.5)}{=} (up + u)|v\rangle = u(p+1)|v\rangle = u(n+1)|v\rangle = (n+1)|uv\rangle,$$

where the third equality follows from the fact that $|v\rangle \in \mathcal{H}_n$ is eigenvector of p corresponding to eigenvalue n, hence, $p|v\rangle = n|v\rangle$. $\square$

Remark 2.8. In the latter definition, a relation between p_i and u_j or between u_i and u_j for $i \neq j$ is not specified in the n-dimensional case ($n > 1$). Clearly, a possible choice is

$$[p_i, u_j] = \delta_{ij} u_j, \tag{2.6}$$

$$[u_i, u_j] = 0 \tag{2.7}$$

However, this assumption could be too restrictive. Namely the second relation should not be a postulate, but rather just a description of a special case.

Proposition 2.9. *Let u be a rising operator of transporter p. Then its spectrum, $\sigma(u) = \{\lambda = \mathrm{e}^{\mathrm{i}\phi} \mid \phi \in \mathbb{R}\}$, is unit circle in $\mathbb{C}$.*

Let $|\psi\rangle$ be a common eigenvector of operators p and D. Then for every $\lambda \in \sigma(u)$ there exists a functional on $\mathcal{H}^\infty$ with the eigenvalue λ, which is of the form

$$\langle\psi_\lambda| = \sum_{n\in\mathbb{Z}} \lambda^{-n} u^n \langle\psi|. \tag{2.8}$$

Proof. Let $\langle\varphi|$ be a continuous linear functional on $\mathcal{H}^\infty$, i.e. $\langle\varphi| \in (\mathcal{H}^\infty)^*$, let $T : \mathcal{H} \longrightarrow \mathcal{H}$, let T^* be smooth. Then operator T acts on $\langle\varphi|$ by

$$\langle T\varphi \mid \psi\rangle = \langle\varphi \mid T^*\psi\rangle \qquad \forall|\psi\rangle \in \mathcal{H}^\infty.$$

Using condition (d) from Definition 2.4 we get that u, u^* are smooth. Then, functional $\langle\psi_\lambda|$ is well defined on $\mathcal{H}^\infty \ni \psi^\infty$:

$$\sum_{n\in\mathbb{Z}}(\lambda^{-n}u^n\langle\psi|)|\psi^\infty\rangle = \sum_{n\in\mathbb{Z}}(\lambda^*)^{-n}\langle\psi \mid (u^*)^n\psi^\infty\rangle,$$

where $|(u^*)^n\psi^\infty\rangle$ is smooth.

Finally, we show that $\langle\psi_\lambda|$ is functional with the eigenvalue λ:

$$\begin{aligned}\langle u\psi_\lambda| &\overset{(2.8)}{=} \Big\langle u\sum_{n\in\mathbb{Z}}\lambda^{-n}u^n\psi\Big| = \sum_{n\in\mathbb{Z}}\lambda^{-n}u^{n+1}\langle\psi| = \\ &= \lambda\sum_{n\in\mathbb{Z}}\lambda^{-(n+1)}u^{n+1}\langle\psi| \overset{m=n+1}{=} \lambda\sum_{m\in\mathbb{Z}}\lambda^{-m}u^m\langle\psi| = \\ &= \lambda\langle\psi_\lambda|. \quad \square\end{aligned}$$

With the help of smooth rising operators we can now construct the algebra of coordinates. We take space of polynomials in u_i and complete it in suitable topology so that all algebra elements are smooth. Commonly studied cases, e.g. n-dimensional torus $\mathbb{T}^n$, can be rephrased in the proposed framework rather easily. We are concerned with the problem of rephrasing the noncommutative torus $\mathbb{T}^2_\theta$.

Example 2.10. Let p and q be two commuting transporters with respective spectra $\sigma_p = \mathbb{Z}$, $\sigma_q = \mathbb{Z}$. The common eigenspaces are non-degenerate (1-dimensional) and are numbered by eigenvalue $n_p = n_q$ for $n_p, n_q < n$ and by (n_p, n_q) for $n_p \geq n$ and $n_q \geq n$. Thus an orthogonal basis for the Hilbert space in terms of eigenvectors of p and q can be given as follows:

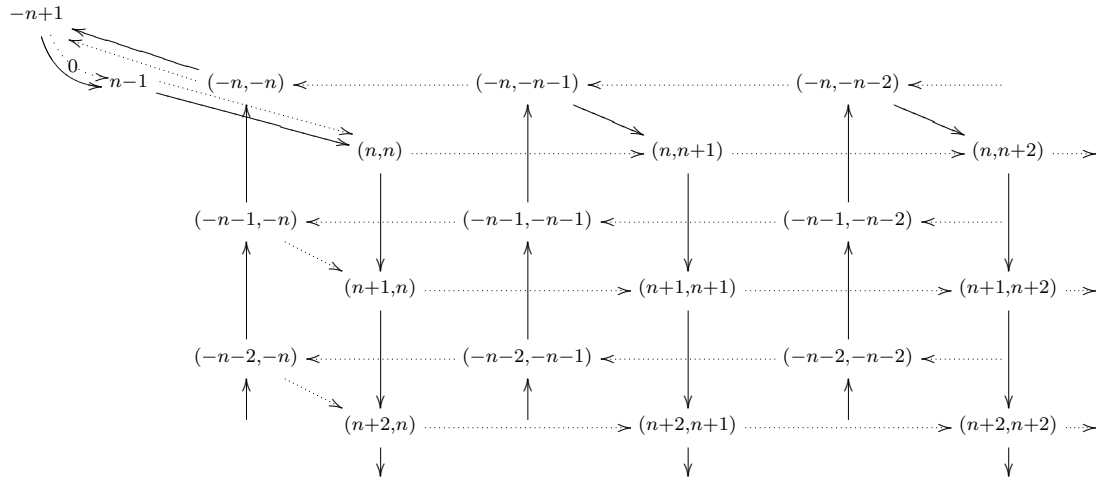
$$\begin{aligned} p|m\rangle &= m|m\rangle && \text{for } m < n, \\ q|m\rangle &= m|m\rangle && \text{for } m < n, \\ p|n_p, n_q\rangle &= n_p|n_p, n_q\rangle && \text{for } \mid n_p \mid \geq n \text{ and } \mid n_q \mid \geq n, \\ q|n_p, n_q\rangle &= n_q|n_p, n_q\rangle && \text{for } \mid n_p \mid \geq n \text{ and } \mid n_q \mid \geq n. \end{aligned}$$

Note that p and q satisfy the properties of a transporter separately for low and high parts of the spectrum but not throughout. The eigenspaces of p for eigenvalues m, $-n < m < n$ are 1-dimensional while the eigenspaces for the other eigenvalues are infinite dimensional. The same is true for q. In particular, p and q are transporters in an asymptotic sense, as forseen in Remark 2.5.

In addition, two ladder operators u, v will be defined:

$$\begin{aligned} u|m\rangle &= |m+1\rangle && \text{for } -n < m < n-1, \\ v|m\rangle &= |m+1\rangle && \text{for } -n < m < n-1, \\ u|n\rangle &= |n, n\rangle, && \\ v|n\rangle &= |n, n\rangle, && \\ u|-n, -n\rangle &= |-n+1\rangle, && \\ v|-n, -n\rangle &= |-n+1\rangle, && \\ u|n_p, n_q\rangle &= |n_p+1, n_q\rangle && \text{for } (n_p < -n \text{ and } n_q \leq -n) \text{ or } (n_p \geq n \text{ and } n_q \geq n), \\ v|n_p, n_q\rangle &= |n_p, n_q+1\rangle && \text{for } (n_p \leq -n \text{ and } n_q < -n) \text{ or } (n_p \geq n \text{ and } n_q \geq n), \\ u|-n, -n_q\rangle &= |n, n_q\rangle && \text{for } n_q < -n, \\ v|-n_p, -n\rangle &= |n_p, n\rangle && \text{for } n_p < -n. \end{aligned}$$

The situation can be summarized by the following diagram, in which vertices denote vectors of the orthogonal basis of the Hilbert space and full arrows (resp. dotted arrows) denote their mapping by u (resp. v):



With these definitions, the space is for low values of the spectrum effectively 1-dimensional (a fuzzy circle) while it is effectively 2-dimensional for values of the spectrum large in their absolute value. Between these two classical regimes there is a concommutativity between u and v so that this is not just a space of classical geometries of different dimensions glued together.

In physical terms, the space in this example is classically 1-dimensional at low energies and classically 2-dimensional at high energies and not a classical space at intermediate energies.

Example 2.11. Let $\mathcal{H}$ denote a separable Hilbert space generated by an orthonormal basis $|n_1, n_2\rangle$, $n_1, n_2 \in \mathbb{Z}$. Let p_1, p_2 be given transporters

$$p_1|n_1, n_2\rangle = n_1|n_1, n_2\rangle,$$
$$p_2|n_1, n_2\rangle = n_2|n_1, n_2\rangle.$$

Let u_1, u_2 be corresponding rising operators defined by

$$u_1|n_1, n_2\rangle = \lambda^{n_2}|n_1 + 1, n_2\rangle,$$
$$u_2|n_1, n_2\rangle = |n_1, n_2 + 1\rangle,$$

with $\lambda = \mathrm{e}^{2\pi \mathrm{i}\,\theta}$ a complex phase. Then we get, by a direct computation,

$$[p_i, u_j] = \delta_{ij} u_j, \qquad [p_i, p_j] = 0, \qquad u_1 u_2 = \lambda u_2 u_1.$$

Rising operators do not commute in this case, cf. Remark 2.8. The Schwartz space $\mathcal{S}(\mathbb{Z}^2)$ of series in u_1, u_2 with rapidly decreasing coefficients generate (represented) algebra of noncommutative torus $\mathbb{T}^2_\theta$. For $\lambda = 1$ this algebra is of course isomorphic to the algebra $\mathcal{C}^\infty(S^1 \times S^1, \mathbb{C})$ of ordinary, commutative torus.

In order to complete defining of the spectral triple a distinguished operator should be added. It can be defined with the help of the transporters. The choice $D = p_1^2 + p_2^2$ corresponds to the Laplace operator. For introducing the Dirac-type operator it is necessary to double the Hilbert space, which allows one to fulfil the requirements of spin geometry, see [7].

A possible physical interpretation of the distinguished operator D identifies it with the Hamiltonian H of the dynamical system. Time evolution is then given by Schrödinger equation

$$\mathrm{i}\,\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle, \qquad \text{with } |\psi\rangle \in \mathcal{H},\ D \equiv H.$$

If D is a Dirac operator, the spin structure needs a separate commentary. That is why the next example is formulated on a spacetime to which Hamiltonian formulation gives a spectral description of space geometry.

Example 2.12. We consider 3-dimensional spacetime with the signature sign $g_{\mu\nu} = (-++)$ of the metric $g_{\mu\nu}$. Compact surfaces at time t_0 are supposed in the form of $\mathbb{T}^2 = S^1 \times S^1$. Clifford bundle over the global hyperbolic spacetime $\mathbb{R} \times \mathbb{T}^2$ is given by the generators γ_μ with

$$\gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu = 2g_{\mu\nu},$$

and it allows to write down the Dirac equation

$$(\gamma^\mu \partial_\mu - m)\psi = 0$$

on the associated spinor bundle $S(\mathbb{T}^2 \times \mathbb{R}) \cong \mathcal{C}^\infty(\mathbb{T}^2 \times \mathbb{R}) \otimes \mathbb{C}^4$. However, we chose the topologically trivial case for simplicity reasons, although $S(\mathbb{T}^2 \times \mathbb{R})$ could bear a nontrivial topological structure.

As we consider the space without curvature, it is possible to choose global coordinates on $S(\mathbb{T}^2 \times \mathbb{R})$ so that the generators γ_μ are constant and they are of the form

$$\gamma_0 = \begin{pmatrix} -\mathrm{i}\,\sigma_2 & 0 \\ 0 & \mathrm{i}\,\sigma_2 \end{pmatrix}, \qquad \gamma_1 = \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_1 \end{pmatrix}, \qquad \gamma_2 = \begin{pmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix},$$

where σ_1, σ_2 and σ_3 are Pauli matrices.

The subspaces of

$$\Gamma = \gamma_0\gamma_1\gamma_2 = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}$$

determine the spinors of respective chirality and dynamics governed by Dirac equation preserves these subspaces. Thus, we can restrict ourselves to chiral spinors with bundles S^L and S^R with

$$S = S^L \oplus S^R, \qquad S^L \cong S^R \cong \mathcal{C}^\infty(\mathbb{T}^2 \times \mathbb{R}) \otimes \mathbb{C}^2.$$

In what follows, we consider S^L only. With the restriction on S^L we get

$$\gamma_0 = -i\sigma_2, \qquad \gamma_1 = \sigma_1, \qquad \gamma_2 = \sigma_3.$$

From Dirac equation modified to the form of Schrödinger equation (A.10) we read of the Hamiltonian

$$H = i\gamma^0(\gamma^k \partial_k - m) = \mathrm{i}\,\sigma_3\partial_1 - i\sigma_1\partial_2 + \sigma_2 m, \tag{2.9}$$

which comprises space Dirac operator. It is the distinguished operator D of the spectral geometry of the torus.

We can easily obtain its spectrum with the corresponding eigenvectors: operator H commutes with H^2 and, consequently, they have common eigenbasis. However, $H^2 = -(\partial_1^2 + \partial_2^2 - m^2)\mathbb{1}_2$ is Laplace operator (except for the sign) with eigenspaces

$$|k_1, k_2\rangle \otimes \mathbb{C}^2 = \mathrm{e}^{\mathrm{i}\,k_1x_1 + \mathrm{i}\,k_2x_2} \otimes \mathbb{C}^2 \tag{2.10}$$

with eigenvalues $m^2 + k_1^2 + k_2^2$, where $k_1, k_2 \in \mathbb{Z}$. The whole subspace corresponding to an eigenvalue λ is given by direct sum of subspaces from (2.10) corresponding to λ.

However, it is supposed tacitly that the length of the torus great circles is equal to 2π. For different lengths, say L_1 and L_2, the eigenspaces are

$$|k_1, k_2\rangle \otimes \mathbb{C}^2 = \mathrm{e}^{2\pi\mathrm{i}(k_1(x_1/L_1) + k_2(x_2/L_2))} \otimes \mathbb{C}^2$$

and the eigenvalues of H^2 are

$$m^2 + \left(\frac{2\pi k_1}{L_1}\right)^2 + \left(\frac{2\pi k_2}{L_2}\right)^2.$$

The eigenfunctions of H belong to the eigenspaces $|k_1, k_2\rangle \otimes \mathbb{C}^2$ of H^2 and have eigenvalue $\pm\sqrt{m^2 + k_1^2 + k_2^2}$. Contrary to the situation with H^2, every eigenvalue $\pm\sqrt{m^2 + k_1^2 + k_2^2}$ of H occurs exactly once in the eigenspace $|k_1, k_2\rangle \otimes \mathbb{C}^2$, as can be proved by a direct computation:

$$H\psi_\pm = \pm\sqrt{m^2 + k_1^2 + k_2^2}\,\psi_\pm, \qquad \text{with} \qquad \psi_\pm = |k_1, k_2\rangle \otimes \begin{pmatrix} k_2 \\ k_1 \pm \sqrt{m^2 + k_1^2 + k_2^2} \end{pmatrix}.$$

We named the orthogonal projector P_+ on direct sum of the eigenspaces H with positive eigenvalue,

$$\bigoplus_{k_1, k_2 \in \mathbb{Z}^2} \left(|k_1, k_2\rangle \otimes \begin{pmatrix} k_2 \\ k_1 + \sqrt{m^2 + k_1^2 + k_2^2} \end{pmatrix} \right)$$

positive energy projector. Denoting $P_- = \mathbb{1} - P_+$ we get

$$H = (P_+ - P_-)\sqrt{H^2}\,.$$

Next, denoting sign of H by $\operatorname{sgn} H = P_+ - P_-$ and absolute value of H by $|H| = \sqrt{H^2}$, we can write down the polar decomposition of H

$$H = \operatorname{sgn} H \cdot |H|. \tag{2.11}$$

In this context, complex structure

$$J = \mathrm{i} \operatorname{sgn} H = \mathrm{i}\, P_+ - \mathrm{i}\, P_- \tag{2.12}$$

bears the physical significace.

Chapter 3

A spectral formulation of non-relativistic QM

Recently, new attempts have appeared to construct quantum theory with minimal assumptions. One by L. Hardy in 2001, see [17], is constructed from the point of view of probability theory. Another by M. Paschke from 2003, called scalar quantum mechanics [32], is inspired by Feynman's proof of the Maxwell equations. Paschke calls it *scalar quantum mechanics* (SQM). He uses purely algebraic definitions of geometric concepts to define quantum mechanics (for one non-relativistic particle) over an arbitrary manifold $\mathcal{Q}$ and shows that his axioms are sufficient to prove the existence of a Hamiltonian with desired properties. More recently, the notion of SQM was discussed in [25] and [33]. However, the necessity of all axioms remains to be elucidated. In this chapter, we justify each axiom as indispensable and present its physical and/or geometric meaning.

The chapter is organized as follows: Section 3.1 recalls the definition and main properties of SQM. In Section 3.2, we study two dynamical systems on the circle ($\mathcal{Q} = S^1$), a simple example of a configuration space with nontrivial topology, i.e. not diffeomorphic to $\mathbb{R}^n$ for some n. We construct a Hamiltonian for each of them. One Hamiltonian is time-independent while the other varies in time. A generalization to $\mathcal{Q} = S^2$ is outlined as well. In Section 3.3, we consider SQM stepwise with one of the axioms violated letting the other axioms hold and we show that a certain essential property of the quantum world fails to hold. In Section 3.4, we illustrate topological obstructions for the existence of the Hamiltonian on multiply connected configuration spaces. More precisely, we show that for such $\mathcal{Q}$ that $H^1(\mathcal{Q}) \neq 0$, there may not exist a Hamiltonian with a potential in $\mathcal{A} = \mathcal{C}_0^\infty(\mathcal{Q})$.

3.1 Scalar quantum mechanics

In this section, we review the concept of SQM as introduced by Paschke in [32]. It is captured by the algebra $\mathcal{A} = \mathcal{C}_0^\infty(\mathcal{Q})$ of smooth real-valued functions on $\mathcal{Q}$ vanishing at infinity, where $\mathcal{Q}$ is a smooth orientable configuration manifold. The observables are constructed from a representation of the algebra on the Hilbert space $\mathcal{H} = L^2(\mathcal{Q}, E)$, i.e. the space of square integrable sections of the complex line bundle $\pi : E \to \mathcal{Q}$. A particular dynamical system is uniquely determined by assigning a time evolution operator U on a corresponding Hilbert space $\mathcal{H}$.

Definition 3.1. Let $\mathcal{A} = \mathcal{C}_0^\infty(\mathcal{Q})$. The system $\{\mathcal{A}_t \mid t \in \mathbb{R}\}$ of unitary representations of the algebra $\mathcal{A}$ is called *scalar quantum mechanics over* $\mathcal{Q}$ if the following conditions hold:

(a) Localizability: Representations of the operators $a_t \in \mathcal{A}_t$ are isomorphic to the representations of the functions $f \in \mathcal{C}_0^\infty(Q)$ on the Hilbert space $\mathcal{H} = L^2(\mathcal{Q}, E)$.

(b) Scalarity: The commutant of $\mathcal{A}_t$, i.e. the set of the operators that commute with all $a_t \in \mathcal{A}_t$, contains merely (complex) functions on $\mathcal{Q}$ and complex multiples of the identity

operator. Thus, $\forall t \in \mathbb{R}$,

$$\mathcal{A}'_t = \overline{(\mathcal{A}_t)_{\mathbb{C}} + \mathbb{C}\mathbb{1}},$$

where $(\mathcal{A}_t)_{\mathbb{C}}$ denotes the complexification of $\mathcal{A}_t$ and is $\overline{(\cdot)}$ is the closure in the weak topology.

(c) Smoothness: The time evolution is smooth with respect to the strong topology and the following holds

$$\mathrm{i}[\mathcal{A}_t, \dot{\mathcal{A}}_t] \subset \mathcal{A}_t, \qquad \forall t \in \mathbb{R}.$$

(d) Positivity: For every self-adjoint operator a_t, the inequality

$$-\mathrm{i}[a_t, \dot{a}_t] \geq 0$$

holds.

(e) Nontriviality: If there exists an operator a_t such that $[a_t, \dot{a}_t] = 0$, then $\dot{a}_t = 0$.

The above axioms do not use a metric structure on $\mathcal{Q}$. Indeed, the metric is characterized by the corresponding SQM and it can be reconstructed from the given time evolution. For all $t \in \mathbb{R}$, it holds (cf. [32, Lemma 3.2]):

$$g_t(\mathrm{d}a_t, \mathrm{d}b_t) = -\mathrm{i}[a_t, \dot{b}_t], \tag{3.1}$$

where g_t is the inverse Riemannian metric and the length scale has been fixed by setting $\hbar = 1$ and $\mathrm{m} = 1$, cf. [32, Remark 3.3].

We also note that this approach corresponds to the Heisenberg picture of the traditional formulation of quantum mechanics—the configuration observables (elements of $\mathcal{A}_t$) depend on t and quantum states (vectors in $\mathcal{H}$) are kept fixed.

Let us recall the main result from [32]:

Theorem 3.2 ([32]). *Under the assumptions* (a)–(e)*, there exists for all $t \in \mathbb{R}$ a unique Riemannian metric g_t given by* (3.1)*, a unique covariant derivative $\nabla(A_t, g_t)$ on the complex line bundle $\pi : E \to \mathcal{Q}$ and a closed one-form $\phi = \varphi_1 \, \mathrm{d}\varphi_2$ such that for all $b_t \in \mathcal{A}_t$ the following holds:*

$$\dot{b}_t = -\mathrm{i}[b_t, \Delta(A_t, g_t)], \tag{3.2}$$

$$\ddot{b}_t = -\mathrm{i}[\dot{b}_t, \Delta(A_t, g_t)] - \mathrm{i}[b_t, \partial\Delta(A_t, g_t)/\partial t] - \mathrm{i}\varphi_1[\varphi_2, \dot{b}_t], \tag{3.3}$$

where

$$\Delta(A_t, g_t) = \frac{1}{2} \sum_{i,j=1}^{\dim \mathcal{Q}} g_t^{ij} \left(-\mathrm{i} \frac{\partial}{\partial q^i} - (A_t)_i \right) \cdot \left(-\mathrm{i} \frac{\partial}{\partial q^j} - (A_t)_j \right)$$

is the covariant Laplacian in local coordinates q^i on $\mathcal{Q}$. If $\phi = \mathrm{d}\varphi_t$ is exact, then there exists a Hamiltonian which is of the form

$$H(t) = \Delta(A_t, g_t) + \varphi_t. \tag{3.4}$$

One may be surprised that the very general axioms of Definition 3.1 specify the admissible dynamics so tightly—spatial derivatives are governed by a second-order Hamiltonian and the time derivatives fulfill Heisenberg equation of motion (3.2) and Newton's law expressed by (3.3).

Lemma 3.3. *Let q denote a local coordinate on the configuration manifold $\mathcal{Q}$. For any vector $\psi(q)$ from a dense subspace $\mathcal{H}_\infty$ of the Hilbert space $\mathcal{H} = L^2(\mathcal{Q}, E)$, the following operator identity holds:*

$$[a_t, \mathrm{d}_q^n] = -\sum_{k=0}^{n-1} \binom{n}{k} (\mathrm{d}_q^{n-k} a_t) \mathrm{d}_q^k \qquad \forall n \in \mathbb{N}, \tag{3.5a}$$

where the differential operators $\mathrm{d}_q^n := \mathrm{d}^n/\mathrm{d}q^n$ are defined on $\mathcal{H}_\infty$ and the operator $a_t(q) \in \mathcal{A}_t$ acts on the states $\psi(q)$ by pointwise multiplication.

The identities for $n = 1$ and 2,

$$[a_t, \mathrm{d}_q] = -\mathrm{d}_q a_t, \tag{3.5b}$$

$$[a_t, \mathrm{d}_q^2] = -\mathrm{d}_q^2 a_t - 2(\mathrm{d}_q a_t)\mathrm{d}_q. \tag{3.5c}$$

are of particular interest and we use them frequently.

Proof. For any $\psi(q) \in \mathcal{H}_\infty$ and $q_0 \in \mathcal{Q}$, we compute

$$\begin{aligned}\Big([a_t(q), \mathrm{d}_q]\psi\Big)(q_0) &= a_t(q_0) \cdot \big(\mathrm{d}_q \psi(q)\big)|_{q=q_0} - \mathrm{d}_q\big(a_t(q) \cdot \psi(q)\big)|_{q=q_0} \\ &= -\big(\mathrm{d}_q a_t(q)\big)|_{q=q_0} \psi(q_0),\end{aligned}$$

which gives (3.5b), and the assertion follows by induction. □

Remark 3.4. SQM provides a compact description of dynamical systems systems formulated in usual QM in a special coordinate system and including many more assumptions. Hence, usual QM is a special case of SQM.

3.2 Examples of SQM over circles and spheres

It is quite instructive to construct a Hamiltonian in some model cases. In order to stress the role of topology in SQM we concentrate on topologically nontrivial configuration spaces.

In the first example, a particularly simple one, we demonstrate the construction of a Hamiltonian, where the topology of $\mathcal{Q}$ does not play any role. Despite this, the example is useful because it serves as an essential ingredient in constructing counterexamples in Section 3.3. Next, we describe the dynamics of a free particle on a sphere, which is a result of a straightforward generalization of the case $\mathcal{Q} = S^1$. The subsequent example illustrates construction of a time-dependent Hamiltonian.

3.2.1 Time-independent case without potentials: a free particle on S^1

Let us fix the setup first. It consists of the algebra $\mathcal{A} = \mathcal{C}^\infty(S^1)$, its representation on the Hilbert space $\mathcal{H} = L^2(S^1, S^1 \times \mathbb{C})$ and the Fourier basis $|m\rangle = \mathrm{e}^{\mathrm{i}m\varphi}, m \in \mathbb{Z}$ on $\mathcal{H}$. The states of the system with respect to this basis have the form $|\psi\rangle = \sum_m c_m |m\rangle$. Finally, the dynamics can be defined by assigning a time evolution operator

$$U(t)|\psi\rangle = \sum_{m\in\mathbb{Z}} c_m \mathrm{e}^{-\mathrm{i}m^2 t} |m\rangle.$$

First, we compute the total time derivative of the arbitrary operator $a_t = U^\dagger(t) \cdot a \cdot U(t)$:

$$\dot{a}_t = U^\dagger(t)[(\mathrm{i}m^2|m\rangle\langle m|), a]U(t). \tag{3.6}$$

If we switch to the coordinate basis and denote $\mathrm{d}_\varphi^n = \mathrm{d}^n/\mathrm{d}\varphi^n$, we can write

$$\dot{a}_t = \mathrm{i}[a_t, \mathrm{d}_\varphi^2]. \tag{3.7}$$

Next, we demonstrate that axioms (a)–(e) are fulfilled:

(a) Localizability is obvious.

(b) Scalarity: As the configuration manifold $\mathcal{Q}$ is compact, $\mathbb{1} \in \mathcal{A}_t$ and we shall prove that $\overline{(\mathcal{A}_t)_\mathbb{C}} = \mathcal{A}_t'$.

We show that $\overline{\mathcal{A}}_t \subset \mathcal{A}_t'$. Let $a \in \overline{\mathcal{A}}_t$ (subscript t being suppressed). Then there exists a sequence $\{a_n\}$ in $\mathcal{A}_t$ such that $a_n \to a$ in the weak topology.

For arbitrary $\psi_1, \psi_2 \in \mathcal{H}$, $b \in \mathcal{A}_t$ we get

$$\begin{aligned}\langle\psi_1|[a,b]|\psi_2\rangle &= \langle\psi_1|[a_n + a - a_n, b]|\psi_2\rangle \\ &= \langle\psi_1|\underbrace{[a_n, b]}_{=0}|\psi_2\rangle + \langle\psi_1|[a - a_n, b]|\psi_2\rangle \\ &= \langle\psi_1|(a - a_n)|b\psi_2\rangle - \langle b^*\psi_1|(a - a_n)|\psi_2\rangle \overset{\mathrm{n}\to\infty}{\longrightarrow} 0\end{aligned}$$

by the definition of convergence in the weak topology, as $b^*\psi_1, b\psi_2 \in \mathcal{H}$.

To sum it up, we get $\langle\psi_1|[a,b]|\psi_2\rangle = 0$ for all $\psi_1, \psi_2 \in \mathcal{H}$ and all $b \in \mathcal{A}_t$. Hence, $a \in \mathcal{A}_t'$.

The reversed inclusion $\overline{\mathcal{A}}_t \supset \mathcal{A}_t'$ follows by standard results from the theory of operator algebras as well, see, e.g., [37].

(c) Smoothness: The time evolution is obviously smooth and

$$\begin{aligned}\mathrm{i}[a_t, \dot{b}_t] = \mathrm{i}[a_t, \mathrm{i}[b_t, \mathrm{d}_\varphi^2]] &\overset{(3.5c)}{=} -[a_t, -\mathrm{d}_\varphi^2 b_t - 2\mathrm{d}_\varphi b_t\,\mathrm{d}_\varphi] = 2[a_t, \mathrm{d}_\varphi b_t\,\mathrm{d}_\varphi] \\ &\overset{(3.5b)}{=} -2\mathrm{d}_\varphi b_t\,\mathrm{d}_\varphi a_t \in \mathcal{A}_t \qquad \forall a_t, b_t \in \mathcal{A}_t.\end{aligned} \tag{3.8}$$

(d) Positivity: Using (3.8), we easily get

$$-\mathrm{i}[a_t, \dot{a}_t] = 2\mathrm{d}_\varphi a_t\,\mathrm{d}_\varphi a_t = 2(\mathrm{d}_\varphi a_t)^2, \tag{3.9}$$

which is nonnegative.

(e) Nontriviality: According to the assumption, we have an operator $a_t \in \mathcal{A}_t$ such that $[a_t, \dot{a}_t] = 0$. We shall show that $\dot{a}_t = 0$ as well. This follows by a simple calculation:

$$\dot{a}_t \overset{(3.7)}{=} \mathrm{i}[a_t, \mathrm{d}_\varphi^2] \overset{(3.5c)}{=} -\mathrm{i}\,\mathrm{d}_\varphi^2 a_t - 2\mathrm{i}(\mathrm{d}_\varphi a_t)\mathrm{d}_\varphi = 0,$$

since $\mathrm{d}_\varphi a_t = 0$ by assumption and (3.9).

We proceed with constructing the metric on $\mathcal{Q}$. Its inverse is given by, cf. [32, Lemma 3.2],

$$g_t(\mathrm{d}b_t, \mathrm{d}c_t) \overset{(3.1)}{=} -\mathrm{i}[b_t, \dot{c}_t] \overset{(3.8)}{=} 2\mathrm{d}_\varphi b_t\,\mathrm{d}_\varphi c_t, \tag{3.10}$$

so the metric $g_t = \frac{1}{2}$ is static.

The total derivative of (3.7) gives us $\ddot{a}_t = -[[a_t, \mathrm{d}_\varphi^2], \mathrm{d}_\varphi^2]$. It is only consistent with (3.3) when $-\mathrm{d}_\varphi^2 = \Delta$. The Hamiltonian is then of the form $H = -\mathrm{d}_\varphi^2 + f_t$, where $\phi = \mathrm{d}f_t$. From (3.3) it follows (cf. also [32, Lemma 3.9]) that $f_t = 0$ and

$$H = -\mathrm{d}_\varphi^2. \tag{3.11}$$

Remark 3.5. If the existence of the Hamiltonian is ensured, we can compute it directly from the given time evolution, as $U(t) = T(\exp[\mathrm{i}\int_0^t H\,\mathrm{d}t])$. It is then of the form

$$H(t) = \mathrm{i}\,\frac{\mathrm{d}U(t)}{\mathrm{d}t} \cdot U(t)^{-1}. \tag{3.12}$$

For the time-independent Hamiltonians, we can utilize Stone's theorem expressed in the formula $U(t) = \exp[\mathrm{i}\,Ht]$. (The Hamiltonian is the generator of the time evolution U.) It is then obtained by a simple calculation and it reads

$$H = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} U(t). \tag{3.13}$$

3.2.2 A free particle on sphere S^2

Assume the algebra $\mathcal{A}_t = \mathcal{C}^\infty(S^2)$, its representation on the Hilbert space $\mathcal{H} = L^2(S^2, S^2 \times \mathbb{C})$ and the Fourier basis $|\ell, m\rangle = Y_{\ell,m}(\theta, \varphi)$, $\ell, m \in \mathbb{Z}$ with $\ell \geq 0, |m| \leq \ell$, on $\mathcal{H}$. Let the dynamics of the system be defined by the time evolution operator

$$U(t)|\psi\rangle = \sum_{\ell,m} c_{\ell,m} \mathrm{e}^{-\mathrm{i}(\ell(\ell+1)/2)t} \, |\ell, m\rangle. \tag{3.14}$$

The total time derivative of the arbitrary operator a_t in the coordinate basis reads

$$\dot{a}_t = \mathrm{i}[a_t, \cot\theta \mathrm{d}_\theta + \mathrm{d}_\theta^2 + \sin^{-2}\theta \mathrm{d}_\varphi^2]. \tag{3.15}$$

Next, we demonstrate that axioms (a)–(e) are fulfilled:

(a) Localizability is obvious.

(b) Scalarity follows by the same arguments as in the preceding section.

(c) Smoothness: The time evolution is obviously smooth and

$$\begin{aligned} \mathrm{i}[a_t, \dot{b}_t] &= \mathrm{i}[a_t, \mathrm{i}[b_t, \cot\theta \mathrm{d}_\theta + \mathrm{d}_\theta^2 + \sin^{-2}\theta \mathrm{d}_\varphi^2]] \\ &= -[a_t, [b_t, \cot\theta]\mathrm{d}_\theta + \cot\theta[b_t, \mathrm{d}_\theta]] - [a_t, [b_t, \mathrm{d}_\theta^2]] \\ &\quad - [a_t, [b_t, \sin^{-2}\theta]\mathrm{d}_\varphi^2 + \sin^{-2}\theta[b_t, \mathrm{d}_\varphi^2]]. \end{aligned} \tag{3.16}$$

The functions $\cot\theta$ and $\sin^{-2}\theta$ commute with any function in $\mathcal{A}_t$. However, as they are unbounded, they are not in the commutant of $\mathcal{A}_t$. Next, $[b_t, \mathrm{d}_\theta] \in \mathcal{A}_t$ and the first term is equal to zero. The second term can be computed analogously like in the preceding section, see (3.8). The third term is treated by combining the above procedures. Summarizing the results, we get

$$\mathrm{i}[a_t, \dot{b}_t] = -2\mathrm{d}_\theta b_t \, \mathrm{d}_\theta a_t - 2\sin^{-2}\theta \mathrm{d}_\varphi b_t \, \mathrm{d}_\varphi a_t \in \mathcal{A}_t, \qquad \forall a_t, b_t \in \mathcal{A}_t. \tag{3.17}$$

This function may appear to be singular at the poles of the sphere, where the spherical coordinates are not defined (formally $\theta \in \{0, \pi\}$). But under closer inspection it turns out to be smoothly extendable to the poles.

(d) Positivity: Using (3.17), we easily get

$$-\mathrm{i}[a_t, \dot{a}_t] = 2(\mathrm{d}_\theta a_t)^2 + 2\sin^{-2}\theta(\mathrm{d}_\varphi a_t)^2 \geq 0. \tag{3.18}$$

(e) Nontriviality: In accordance with the assumption, we have an operator $a_t \in \mathcal{A}_t$ such that $[a_t, \dot{a}_t] = 0$. With (3.18), it follows that $\mathrm{d}_\theta a_t = 0 = \mathrm{d}_\varphi a_t$ and the assertion $\dot{a}_t = 0$ follows by a simple calculation:

$$\begin{aligned} \dot{a}_t &\overset{(3.15)}{=} \mathrm{i}[a_t, \cot\theta \mathrm{d}_\theta] + \mathrm{i}[a_t, \mathrm{d}_\theta^2] + \mathrm{i}[a_t, \sin^{-2}\theta \mathrm{d}_\varphi^2] \\ &\overset{(3.5\mathrm{bc})}{=} -\mathrm{i}\cot\theta \mathrm{d}_\theta a_t - \mathrm{i}(\mathrm{d}_\theta^2 a_t + 2\mathrm{d}_\theta a_t \, \mathrm{d}_\theta) - \mathrm{i}\sin^{-2}\theta(\mathrm{d}_\varphi^2 a_t + 2\mathrm{d}_\varphi a_t \, \mathrm{d}_\varphi) \\ &= 0. \end{aligned}$$

We proceed with constructing the metric on $\mathcal{Q}$ again. Its inverse is given by, cf. [32, Lemma 3.2],

$$g_t(\mathrm{d}b_t, \mathrm{d}c_t) \overset{(3.1)}{=} -\mathrm{i}[b_t, \dot{c}_t] \overset{(3.17)}{=} 2\mathrm{d}_\theta b_t \, \mathrm{d}_\theta c_t + 2\sin^{-2}\theta \mathrm{d}_\varphi b_t \, \mathrm{d}_\varphi c_t, \tag{3.19}$$

and

$$g_{ij} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & \sin^2\theta \end{pmatrix}.$$

The Laplacian $\Delta(a_t) = -\frac{1}{2}g^{\mu\nu}\nabla_\mu\nabla_\nu(a_t) = -\cot\theta \mathrm{d}_\theta a_t - \mathrm{d}_\theta^2 a_t - \sin^{-2}\theta \mathrm{d}_\varphi^2 a_t$ corresponding to this metric expressed in spherical harmonics is

$$\Delta|\ell, m\rangle = \frac{\ell(\ell+1)}{2}|\ell, m\rangle.$$

It coincides with the Hamiltonian of the time evolution (3.14).

We have seen that in terms of SQM this is an easy generalization of the preceding case. Particularly in comparison with the usual derivation, cf. [40, Chapter I], it is obvious that SQM offers a direct and concise description of systems, which must be solved in the usual description with special techniques.

SQM on homogeneous spaces Moreover, we show that SQM on S^2 can be easily rephrased in the language of harmonic analysis on compact Lie groups and their homogeneous spaces, thus pointing to the essentials of this more general setting. The sphere S^2 is a homogeneous space $O(3)/O(2)$ with the action of the compact Lie group $O(3)$ of orthogonal transformations on $\mathbb{R}^3$. The algebra $\mathcal{A} = C^\infty(S^2)$ consists of smooth vectors under the induced action on the representation Hilbert space $\mathcal{H} = L^2(S^2)$ built upon the Haar measure. This compares to the localizability axiom.

Moreover, we can naturally construct from this representation a Fourier basis in $\mathcal{H}$ determined by irreducible representations. They possess a quadratic Casimir operator, which is just the Laplace operator. Indeed, by theorem 3.2 it differs from the Hamiltonian by not more than a function $\varphi_t \in \mathcal{A}_t$, which for a free particle is equal to zero. Thus, the Casimir operator exactly generates the time evolution.

In this framework, SQM can be easily formulated on S^n for any $n \geq 2$; for details see [18].

3.2.3 A system with a time-dependent Hamiltonian: a particle on an expanding circle

Now, let the dynamics of the system be defined by

$$U(t) = \exp[-\mathrm{i}m^2 G_{(\mathrm{A})}(t)],$$

where $G_{(\mathrm{A})}$ is an arbitrary increasing function of time. We use Remark 3.5, especially (3.12), to compute the Hamiltonian. In coordinate representation, it is given by $H(t) = -g_{(\mathrm{A})}\mathrm{d}_\varphi^2$, where $g_{(\mathrm{A})}(t) = \mathrm{d}G_{(\mathrm{A})}(t)/\mathrm{d}t$. Now, we can compute the total time derivative of an arbitrary operator a_t, cf. (3.2),

$$\dot{a}_t = \mathrm{i}\, g_{(\mathrm{A})}[a_t, \mathrm{d}_\varphi^2]. \tag{3.20}$$

It is obvious that axioms (a)–(e) hold, we shall only comment briefly the positivity axiom: The expression

$$-\mathrm{i}[a_t, \dot{a}_t] \overset{(3.8)}{=} 2g_{(\mathrm{A})}\mathrm{d}_\varphi a_t\, \mathrm{d}_\varphi a_t = 2g_{(\mathrm{A})}(\mathrm{d}_\varphi a_t)^2 \tag{3.21}$$

is nonnegative if $g_{(\mathrm{A})}$ is nonnegative, that is, if $G_{(\mathrm{A})}$ is increasing, which we assume.

Remark 3.6. The function $g_{(\mathrm{A})}$ is the inverse Riemannian metric on $\mathcal{Q}$ and it governs the velocity of expansion of the circle,

$$g_{(\mathrm{A})}(t) = \frac{1}{2R^2(t)},$$

where R is the radius of the circle $\mathcal{Q}$.

Remark 3.7. A particle on an expanding sphere can be defined analogously.

3.3 The necessity of the axioms of SQM

In this section, we show that none of the axioms of SQM can be dropped. We consider SQM stepwise with just one of them violated and in all four cases we find a significant property of the quantum world which fails to hold.

The localizability axiom only sets up the framework of smooth manifolds, C^*-algebras and their representations on Hilbert spaces. We work mainly on one-dimensional manifolds S^1 and $\mathbb{R}$ here.

We keep the notation of Section 3.2.1 (the objects with subscript t or without subscript), because we utilize it in the following constructions. When we need a simpler notation, the subscript t is dropped.

3.3.1 The scalarity axiom implies Newton's law

The axiom is to be broken by choosing a "larger" Hilbert space, where an operator exists that commutes with all $a_t \in \mathcal{A}_t$, but that does not fall into $\overline{\mathcal{A}}_t$. Thus, we suppose that

$$\mathcal{A}'_t \supsetneq \overline{\mathcal{A}}_t. \tag{3.22}$$

We construct such system by modifying the example of Section 3.2.1 as follows. We consider the algebra $\mathcal{A} = \mathcal{C}^\infty(S^1)$ represented on the Hilbert space $\mathcal{H}_{(1)} = \mathcal{H} \otimes \mathbb{C}^2 = L^2(S^1, S^1 \times \mathbb{C}) \otimes \mathbb{C}^2$ and denote the representation simply by $\mathcal{A}_{(1)} = \mathcal{A}_t \otimes \mathbb{1}_{\mathbb{C}^2}$. Note that all operators of Section 3.2.1 can be expressed in the form $\mathcal{A}_{(1)} \ni a_{(1)} = a_t \otimes \mathbb{1}_{\mathbb{C}^2}$, where a_t is represented on $\mathcal{H}$.

The dynamics is defined with the help of the time evolution operator $U(t)$ of Section 3.2.1. It reads $U_{(1)}(t) = (U \otimes U_{\mathbb{C}^2})(t) = \mathrm{e}^{-\mathrm{i}m^2 t} \otimes \mathrm{e}^{-\mathrm{i}f^j(t)\sigma_j}$, where f^j are arbitrary functions and the summation convention on index j has been used. According to Remark 3.5, we can compute the Hamiltonian from (3.12):

$$\begin{aligned} H_{(1)}(t) &= \mathrm{i}\,\frac{\mathrm{d}(U \otimes U_{\mathbb{C}^2})}{\mathrm{d}t} \cdot (U \otimes U_{\mathbb{C}^2})^{-1} \\ &= \mathrm{i}\,\frac{\mathrm{d}U}{\mathrm{d}t} \cdot U^{-1} \otimes U_{\mathbb{C}^2} \cdot (U_{\mathbb{C}^2})^{-1} + \mathrm{i}\,U \cdot U^{-1} \otimes \frac{\mathrm{d}U_{\mathbb{C}^2}}{\mathrm{d}t} \cdot (U_{\mathbb{C}^2})^{-1} \\ &= H \otimes \mathbb{1}_{\mathbb{C}^2} + \mathbb{1} \otimes H_{\mathbb{C}^2}, \end{aligned}$$

where $H_{\mathbb{C}^2} = \dot{f}^j(t)\sigma_j$. We only demand that the f's are Hermitian operators, i.e., real functions on $\mathbb{C}$. We note that $\dot{H}_{(1)} = \mathbb{1} \otimes \ddot{f}^j(t)\sigma_j$.

However, the rest of the axioms of SQM is fulfilled. Let us demonstrate it.

(c) Smoothness: The time evolution is obviously smooth and the required inclusion follows from (3.8):

$$\begin{aligned} \mathrm{i}[a_{(1)}, \dot{b}_{(1)}] &= \mathrm{i}[a_{(1)}, \mathrm{i}[b_{(1)}, H_{(1)}]] \\ &= -[a_{(1)}, [b_t \otimes \mathbb{1}_{\mathbb{C}^2}, H \otimes \mathbb{1}_{\mathbb{C}^2} + \mathbb{1} \otimes H_{\mathbb{C}^2}]] \\ &= \mathrm{i}[a_t, \underbrace{\mathrm{i}[b_t, H]}_{=\dot{b}_t}] \otimes \mathbb{1}_{\mathbb{C}^2} - [a_{(1)}, \underbrace{[b_t \otimes \mathbb{1}_{\mathbb{C}^2}, \mathbb{1} \otimes H_{\mathbb{C}^2}]}_{=0}] \\ &\overset{(3.8)}{=} -2\mathrm{d}_\varphi b_t\, \mathrm{d}_\varphi a_t \otimes \mathbb{1}_{\mathbb{C}^2} \in \mathcal{A}_{(1)} \qquad \forall a_{(1)}, b_{(1)} \in \mathcal{A}_{(1)}. \end{aligned} \tag{3.23}$$

(d) Positivity: Using (3.23) and (3.8), we easily get

$$-\mathrm{i}[a_{(1)}, \dot{a}_{(1)}] = -\mathrm{i}[a_t, \dot{a}_t] \otimes \mathbb{1}_{\mathbb{C}^2} = 2(\mathrm{d}_\varphi a_t)^2 \otimes \mathbb{1}_{\mathbb{C}^2} \geq 0.$$

(e) Nontriviality follows by the same reasoning as in the example of Section 3.2.1, since $0 \otimes \mathbb{1}_{\mathbb{C}^2} = 0_{(1)}$.

We interpret Newton's law as a rule assuring that the second time derivative of any operator b is fully determined by b and $\dot{b}$. For a choice $b = q_i$, with a local coordinate q_i, the interpretation is particularly apparent, as Newton's law is usually expressed in the form $\ddot{q}_i = F(t, q, \dot{q})$ for some function F. In this sense, equation (3.3) can be considered as Newton's law.

An operator $b_{(1)}$ on $\mathcal{H}_{(1)}$ that illustrates the effects of the condition (3.22), i.e. $b_{(1)} \in \mathcal{A}'_{(1)} \setminus \overline{\mathcal{A}_{(1)}}$, can be constructed with the help of an arbitrary Pauli matrix σ_i ($i = 1, 2, 3$). It is of the form $b_{(1)} = b_t \otimes \sigma_i$, where b_t is again represented on $\mathcal{H}$.

Let us compute its time derivative. From (3.2), it follows that

$$\dot{b}_{(1)} = -\mathrm{i}[b_{(1)}, H_{(1)}] = \mathrm{i}[b_t, \mathrm{d}_\varphi^2] \otimes \sigma_i + 2\epsilon_{ijk}\, b_t \otimes \dot{f}^j \sigma_k, \tag{3.24}$$

where the summation convention on indices j, k has been used. The second time derivative can be obtained by a tedious calculation

$$\begin{aligned}
\ddot{b}_{(1)} &= -\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}[b_{(1)}, H_{(1)}] \\
&= -\mathrm{i}[\mathrm{i}[b_t, \mathrm{d}_\varphi^2] \otimes \sigma_i, -\mathrm{d}_\varphi^2 \otimes \mathbb{1}_{\mathbb{C}^2}] - \mathrm{i}[\mathrm{i}[b_t, \mathrm{d}_\varphi^2] \otimes \sigma_i, \mathbb{1} \otimes \dot{f}^j \sigma_j] \\
&\quad - \mathrm{i}[2\epsilon_{ijk}\, b_t \otimes \dot{f}^j \sigma_k, -\mathrm{d}_\varphi^2 \otimes \mathbb{1}_{\mathbb{C}^2}] - \mathrm{i}[2\epsilon_{ijk}\, b_t \otimes \dot{f}^j \sigma_k, \mathbb{1} \otimes \dot{f}^m \sigma_m] \\
&\quad - \mathrm{i}[b_t \otimes \sigma_i, \mathbb{1} \otimes \ddot{f}^j \sigma_j],
\end{aligned}$$

using (3.24), and this becomes

$$\begin{aligned}
\ddot{b}_{(1)} =& -[[b_t, \mathrm{d}_\varphi^2], \mathrm{d}_\varphi^2] \otimes \sigma_i + 4\mathrm{i}\,\epsilon_{ijk}\,[b_t, \mathrm{d}_\varphi^2] \otimes \dot{f}^j \sigma_k \\
&+ 4(\delta_{im}\delta_{jk} - \delta_{ik}\delta_{jm})\, b_t \otimes \dot{f}^j \dot{f}^m \sigma_k + 2\epsilon_{ijk}\, b_t \otimes \ddot{f}^j \sigma_k,
\end{aligned} \tag{3.25}$$

(summation over j, k, m).

There remains the second derivative of the function f (steming from $H_{\mathbb{C}^2}$) that cannot be determined from $b_{(1)}$ and $\dot{b}_{(1)}$. Hence, we cannot express the second time derivative of an arbitrary operator $b_{(1)}$ from the first and zeroth one and $\ddot{b}_{(1)}$ cannot be expressed in the form of Newton's law (3.3).

3.3.2 The smoothness axiom restricts order of the Hamiltonian

The smoothness condition is also called the second-order condition, because it guarantees that the Hamiltonian is of second-order at the most. Indeed, a violation of this axiom could admit too wild time evolutions of the systems, e.g., such that are governed by a higher-order Hamiltonian. Whether this is indeed the case, hinges upon to what degree such examples are ruled out by one of the other axioms, positivity. The impact of the positivity axiom is highly nontrivial (for results on the positivity of commutators see [23, 22, 15]). We are thus forced by the present knowledge on this problem to relax the positivity condition and will in fact show that it cannot be satisfied, e.g. by any differential operator of order higher than 2.

We construct a system on the bundle $\pi : \mathbb{R} \times \mathbb{C} \longrightarrow \mathbb{R}$ that is determined by the time evolution operator $U_{(2)}(t) = \exp[\mathrm{i}t \cdot \exp[-p^2]]$. We immediately see that this time evolution is generated by the Hamiltonian

$$H_{(2)} = \mathrm{e}^{-p^2} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} p^{2n},$$

which is "of order ∞". This Hamiltonian is a well defined self-adjoint operator on the Schwartz space $\mathcal{S}(\mathbb{R})$, the space of smooth complex functions f on $\mathbb{R}$ such that

$$\lim_{|x|\to\infty} |x|^m f^{(n)}(x) = 0, \qquad \forall m, n = 0, 1, 2, \ldots,$$

see [36, Section V.3]. It follows from the well-known result that the Fourier transformation is an isometry of $\mathcal{S}(\mathbb{R})$.

We recall that $\mathcal{S}(\mathbb{R})$ is dense in $L^2(\mathbb{R}, \mathbb{R}\times\mathbb{C})$. According to Plancherel's theorem, see [36, Theorem IX.6], the Fourier transform map on $\mathcal{S}(\mathbb{R})$ extends uniquely to a linear isometry of $L^2(\mathbb{R})$ and, consequently, $H_{(2)}$ is a well-defined operator on entire Hilbert space $\mathcal{H}$.

In order to illustrate the smoothness requirement for this particular system, we shall compute the time derivative of an arbitrary operator $a_{(2)} \in \mathcal{A}_{(2)} = \mathcal{C}_0^\infty(\mathbb{R})$,

$$\dot{a}_{(2)}(x) = -\mathrm{i}[a_{(2)}(x), H_{(2)}] = -\mathrm{i}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}[a_{(2)}(x), p^{2n}].$$

In the coordinate representation, where $p|\psi\rangle = -\mathrm{i}\,\mathrm{d}_x\psi$, we get

$$\begin{aligned}\dot{a}_{(2)}(x) &= -\mathrm{i}\sum_{n=0}^{\infty}\frac{(-1)^n(-\mathrm{i})^{2n}}{n!}[a_{(2)}(x), \mathrm{d}_x^{2n}]\\ &\overset{(3.5a)}{=} \sum_{n=0}^{\infty}\sum_{r=0}^{2n-1}\frac{(-1)^{n+1}(-\mathrm{i})^{2n+1}}{n!}\binom{2n}{r}(\mathrm{d}_x^{2n-r}a_{(2)})\mathrm{d}_x^r,\end{aligned}$$

where $(-1)^{n+1}(-\mathrm{i})^{2n+1} = -\mathrm{i}$ for all $n \in \mathbb{N}$. We proceed with computing the commutator $\mathrm{i}[b_{(2)}, \dot{a}_{(2)}]$:

$$\begin{aligned}\mathrm{i}[b_{(2)}, \dot{a}_{(2)}] &= \mathrm{i}\sum_{n=0}^{\infty}\sum_{r=0}^{2n-1}\frac{(-\mathrm{i})}{n!}\binom{2n}{r}[b_{(2)}, (\mathrm{d}_x^{2n-r}a_{(2)})\mathrm{d}_x^r]\\ &\overset{(3.5a)}{=} -\sum_{n=0}^{\infty}\sum_{r=0}^{2n-1}\sum_{s=0}^{r-1}\frac{1}{n!}\binom{2n}{r}\binom{r}{s}(\mathrm{d}_x^{2n-r}a_{(2)})(\mathrm{d}_x^{r-s}b_{(2)})\mathrm{d}_x^s\end{aligned} \tag{3.26}$$

and then show that the latter expression does not fall into $\mathcal{A}_{(2)}$. For this, it is sufficient to outline that it does not commute with an operator $c_{(2)} \in \mathcal{A}_{(2)}$. But this is obvious, as the commutator cuts the order of free derivatives by one and the sum remains to be infinite.

Should it fall into $\mathcal{A}_{(2)}$, the summation index s would have to be at the most equal to 1 (so as n) and we get that $H_{(2)}$ would have to be of second order.

However, the operator defined by (3.26) does not commute even after an arbitrary finite number of commutations with operators from $\mathcal{A}_{(2)}$!

Next, we briefly comment the fact that other axioms apart from positivity axiom are fulfilled:

(a) Localizability is obvious.

(b) Scalarity follows by the same arguments as in Section 3.2.1.

(d) Positivity: The positivity requirement was relaxed in this example due to the above comments.

Let us note that it follows from (3.5a) that any differential operator of order $n \geq 3$ can not fulfill positivity requirement, as the first and the second commutator are sums of differential operators of order i for all $i \in \{0, 1, \ldots, n-1\}$ and they both contain operator d_x with spectrum equal to $\mathbb{R}$, cf. also remarkable work of Kato [23]. However, our example shows that positivity of the Hamiltonian is not sufficient for the positivity axiom to hold.

It is clear from literature that we are concerned with a delicate question. Research of positive commutators started in 1960's by pioneering works of Putnam and Kato. In 1978 Reed and Simon [36, vol. IV, p. 158] admitted that it is "not easy to construct directly" any pairs of operators a, H such that $-\mathrm{i}[a, H] \geq 0$. As a consequence of the attempts to understand the spectrum of the Hamiltonian in the scattering theory the positive commutator method of Mourre was established, cf. [22]. Its rapid development has continued since early 1980's, cf. Georgescu, Gérard and Møller [15]. This theory is not applicable in our case, as they look for *any* operator

for which the commutator with H is positive whereas we need *every* multiplication operator to give positive commutator with H. The question remains open for a further research.

(e) Nontriviality: In accordance with the assumption, we have an operator $a_{(2)}(x) \in \mathcal{A}_{(2)}$ such that $[a_{(2)}(x), \dot{a}_{(2)}(x)] = -\mathrm{i}[a_{(2)}(x), [a_{(2)}(x), H_{(2)}]] = 0$. As $H_{(2)} = f(p)$ is a differential operator of order $n > 2$, it is only possible if $a_{(2)}(x) = \text{const}$, cf. [23, Theorem I]. As $a \in \mathcal{C}_0^\infty(\mathbb{R})$, we get $a_{(2)}(x) = 0$. But then also $\dot{a}_{(2)}(x) = 0$.

The smoothness axiom also specifies the form of the canonical commutation relations. This axiom generalizes Feynman's assumption of the standard Heisenberg relation $\mathrm{m}[x_j, \dot{x}_k] = i\hbar\delta_{jk}$, see [13, eq. (3)]. It relaxes the particular form of the latter commutator and we only require that it is a function of operators from $\mathcal{A}_t$, i.e. operators which act by pointwise multiplication. In the global coordinates $(x_i)_{i=1,\dots,n}$ on $\mathbb{R}^n$, we recover the Heisenberg relation back.

3.3.3 The consequences of positivity and nontriviality

The axioms of positivity and nontriviality are closely connected. They determine positive definiteness of the metric and proper boundedness of the spectrum of the corresponding Hamiltonian. They are discussed first separately but also violated concurrently to produce an example exhibiting an indefinite metric, which is interesting on its own right.

The positivity axiom ensures positive definite metric

The positivity axiom is easily broken by the time reversal in the ordinary SQM system, e.g. that of Section 3.2.1. The time evolution operator is then given by

$$U_{(3)}(t)|\psi\rangle = \sum_{m\in\mathbb{Z}} c_m \mathrm{e}^{\mathrm{i}m^2 t}\,|m\rangle.$$

It is of course generated by a Hamiltonian

$$H_{(3)} = \mathrm{d}_\varphi^2 \tag{3.27}$$

and all axioms apart from (d) are fulfilled.

Let us illustrate the violation of positivity. The total time derivative of an operator a_t is given by $\dot{a}_t = -\mathrm{i}[a_t, \mathrm{d}_\varphi^2]$ and we easily get that

$$-\mathrm{i}[a_t, \dot{a}_t] = -2(\mathrm{d}_\varphi a_t)^2 \leq 0. \tag{3.28}$$

We proceed with constructing the metric on $\mathcal{Q}$. Its inverse is given by

$$g_{(3)}(\mathrm{d}b_t, \mathrm{d}c_t) = -\mathrm{i}[b_t, \dot{c}_t] = -2\mathrm{d}_\varphi b_t\, \mathrm{d}_\varphi c_t, \tag{3.29}$$

so the metric $g_{(3)} = -\frac{1}{2}$ is negative definite. Finally, let us note that spectrum of $H_{(3)}$ is semi-bounded from above and by a proper choice of time direction one can always achieve positivity.

The nontriviality axiom: trivial means unquantized

The nontriviality condition guarantees that the Hamiltonian is at least of second order. We shall construct a model where there exists an operator $a_t \in \mathcal{A}_t$ such that

$$[a_t, \dot{a}_t] = 0 \quad \text{and} \quad \dot{a}_t \neq 0. \tag{3.30}$$

We consider SQM over $\mathbb{R}$, i.e. $\mathcal{A}_{(4)} = \mathcal{C}_0^\infty(\mathbb{R}), \mathcal{H}_{(4)} = L^2(\mathbb{R}, \mathbb{R}\times\mathbb{C})$, with the time evolution given by $U_{(4)}(t)|\psi\rangle = \psi(x-t)$. Let us compute its generator:

$$\psi(x-t) = \sum_{k=0}^{\infty} \frac{(-t)^k}{k!}\frac{\mathrm{d}^k\psi}{\mathrm{d}x^k} = \mathrm{e}^{-t\mathrm{d}_x}\,\psi(x).$$

According to (3.13), it is generated by the Hamiltonian $H_{(4)} = -\mathrm{i}\,\mathrm{d}_x$. As in the preceding sections, we compute the time derivative $\dot{a}_{(4)}$ of an operator $a_{(4)}$,

$$\dot{a}_{(4)} = -\mathrm{i}[a_{(4)}, -\mathrm{i}\,\mathrm{d}_x] = \mathrm{d}_x a_{(4)}, \tag{3.31}$$

and test the other SQM-axioms:

(b) Scalarity: The assertion follows by the same arguments as in Section 3.2.1.

(c) Smoothness: The time evolution of the system is obviously smooth and for every $a_{(4)}, b_{(4)} \in \mathcal{A}_{(4)}$ it holds

$$\mathrm{i}[a_{(4)}, \dot{b}_{(4)}] = \mathrm{i}[a_{(4)}, \mathrm{d}_x b_{(4)}] = 0 \in \mathcal{A}_{(4)}, \tag{3.32}$$

because $\mathrm{d}_x b_{(4)} \in \mathcal{A}_{(4)}$ and because $\mathcal{A}_{(4)}$ is commutative.

(d) Positivity: Using (3.32), we easily get $-\mathrm{i}[a_{(4)}, \dot{a}_{(4)}] = 0 \geq 0$.

We illustrate the behavior of the system on the position operator $x_{(4)}$. From (3.31) it follows that $\dot{x}_{(4)} = \mathrm{d}_x x_{(4)} = \mathbb{1}$ and the momentum operator is given by $p_{(4)} = \mathrm{m}\mathbb{1}$. Let us compute the canonical commutation relation:

$$[x_{(4)}, p_{(4)}] = \mathrm{m}[x_{(4)}, \mathbb{1}] = 0, \tag{3.33}$$

the position operator commutes with the momentum operator and, therefore, this model describes an unquantized mechanical system.

Let us try to construct the Hamiltonian from the definition. From (3.32) it follows that the metric $g_{(4)}$ is degenerate, even identically zero. Thus, the construction of the covariant Laplacian breaks down, $H_{(4)}$ is not of the form (3.4) and its spectrum $\sigma(H_{(4)}) = \mathbb{R}$ has neither a lower nor an upper bound!

Violating both positivity and nontriviality allows indefinite metrics

We discuss SQM on the torus $\mathbb{T} = S^1 \times S^1$ as a product of two SQM over the circle that has been worked out in Section 3.2.1. Thus, we consider the algebra $\mathcal{A}_{(5)} = \mathcal{C}^\infty(\mathbb{T})$ represented on $\mathcal{H}_{(5)} = L^2(\mathbb{T}, \mathbb{T} \times \mathbb{C})$. The product states are of the form $|\psi\rangle = \sum_{m,n} c_{mn}|m,n\rangle$, where $|m,n\rangle = |\mathrm{e}^{\mathrm{i}m\phi_1}, \mathrm{e}^{\mathrm{i}n\phi_2}\rangle$ and ϕ_1 and ϕ_2 denote the angular coordinates on the corresponding circles.

Let the dynamics of the system be defined by the time evolution operator

$$U_{(5)}(t)|\psi\rangle = \sum_{m,n\in\mathbb{Z}} c_{mn}(\phi_1, \phi_2)\mathrm{e}^{-\mathrm{i}m^2 t}\,\mathrm{e}^{\mathrm{i}n^2 t}\,|m,n\rangle.$$

As in Section 3.2.1, we first compute the total time derivative of an arbitrary operator $a_{(5)}(\phi_1, \phi_2)$ that is by virtue of (3.6) and (3.7)

$$\dot{a}_{(5)} = \mathrm{i}[a_{(5)}, \mathrm{d}^2_{\phi_1}] - \mathrm{i}[a_{(5)}, \mathrm{d}^2_{\phi_2}]. \tag{3.34}$$

So we can construct a Hamiltonian with the same procedure as in Section 3.2.1 or compute it with the help of Remark 3.5, in particular by eqn. (3.13). Be it this way or the other, it is of the form $H_{(5)} = \mathrm{d}^2_{\phi_2} - \mathrm{d}^2_{\phi_1}$.

Next, we demonstrate that other axioms are fulfilled. In doing so, let us suppress the index $_{(5)}$.

(b) Scalarity: The assertion follows by the same argument as in the preceding sections.

(c) Smoothness: The time evolution is obviously smooth and $\forall a, b \in \mathcal{A}$ it holds

$$\begin{aligned}
\mathrm{i}[a, \dot{b}] &= \mathrm{i}[a, \mathrm{i}[b, \mathrm{d}^2_{\phi_1}] - \mathrm{i}[b, \mathrm{d}^2_{\phi_2}]] \\
&= -[a, -\mathrm{d}^2_{\phi_1} b - 2\mathrm{d}_{\phi_1} b\,\mathrm{d}_{\phi_1}] + [a, -\mathrm{d}^2_{\phi_2} b - 2\mathrm{d}_{\phi_2} b\,\mathrm{d}_{\phi_2}] \\
&= \underbrace{[a, \mathrm{d}^2_{\phi_1} b]}_{=0} + 2\underbrace{[a, \mathrm{d}_{\phi_1} b\,\mathrm{d}_{\phi_1}]}_{\in\mathcal{A}} - \underbrace{[a, \mathrm{d}^2_{\phi_2} b]}_{=0} - 2\underbrace{[a, \mathrm{d}_{\phi_2} b\,\mathrm{d}_{\phi_2}]}_{\in\mathcal{A}} \\
&= -2\mathrm{d}_{\phi_1} b\,\mathrm{d}_{\phi_1} a + 2\mathrm{d}_{\phi_2} b\,\mathrm{d}_{\phi_2} a \in \mathcal{A}.
\end{aligned} \tag{3.35}$$

With the help of the smoothness axiom (3.35), we can easily illustrate the violation of the axioms and its consequences.

The positivity condition

$$-\mathrm{i}[a,\dot{a}] = 2(\mathrm{d}_{\phi_1}a)^2 - 2(\mathrm{d}_{\phi_2}a)^2 \tag{3.36}$$

results obviously indefinite. Let us consider an operator a with $[a,\dot{a}]=0$. We can apply (3.35) to get

$$\dot{a} = -2(\mathrm{d}_{\phi_1}a)\mathrm{d}_{\phi_1} + 2(\mathrm{d}_{\phi_2}a)\mathrm{d}_{\phi_2},$$

which is zero only if $\mathrm{d}_{\phi_1}a = 0 = \mathrm{d}_{\phi_2}a$. This describes a subset of operators fulfilling the nontriviality axiom.

Nevertheless, we can construct a metric on $\mathbb{T}$, only it fails to be Riemannian. More precisely, $(\mathbb{T}, g_{\mathbb{T}})$ is a pseudo-Riemannian manifold with metric

$$g_{\mathbb{T}} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix},$$

and the spectrum of the Hamiltonian $H_{(5)}$ has neither a lower nor an upper bound!

3.4 Topological aspects of SQM on multiply connected configuration spaces

We have already seen an example of a system on a multiply connected space, namely on S^1, see Section 3.2.1, but in the case of a Hamiltonian without potentials, the nontrivial topology of the configuration manifold does not play any role.

The construction presented here has been inspired by one of the most famous experiments showing topological effects in quantum theory, namely the Aharonov–Bohm effect in its electric form, see analysis by W. Moreau and D.K. Ross in [30]. Thus, the results have clear physical background and consequences.

We again modify the example of Section 3.2.1 in this construction; we keep the configuration manifold $\mathcal{Q} = S^1$, the algebra of observables $\mathcal{A} = \mathcal{C}^\infty(S^1)$ and its representation on the Hilbert space $\mathcal{H} = L^2(S^1, S^1 \times \mathbb{C})$ and set up the time evolution so as to violate the existence of a Hamiltonian with a potential in $\mathcal{A}_t$. It reads:

$$U(t) = \sum_{m\in\mathbb{Z}} \mathrm{e}^{\mathrm{i}E_m t}\, |m\rangle\langle m|.$$

Let the states of the system with respect to the coordinate basis be of the form

$$\psi_m(\varphi) = \langle \varphi \mid m\rangle = C_1\,\mathrm{Ai}(\varphi - E_m) + C_2\,\mathrm{Bi}(\varphi - E_m), \tag{3.37}$$

where Ai and Bi are Airy functions, see, e.g., [1, 43]. Here, on $\mathcal{Q} = S^1$, the wave functions have to fulfill the following conditions:

$$\psi_m(0) = \psi_m(2\pi), \tag{3.38a}$$

$$\psi'_m(0) = \psi'_m(2\pi). \tag{3.38b}$$

Provided these conditions on E hold, the spectrum of H is discrete as in the case without potential, cf. Section 3.2.1. However, the spectrum cannot be given by a simple closed formula. The Hamiltonian is then of the form $\widehat{H} = \widehat{P}^2 + \widehat{X}$, where $\widehat{X}$ is the local potential of a constant one-form. Note, that $\widehat{X} \notin \mathcal{A}_t = \mathcal{C}^\infty(S^1)$, as it is not continuous in $\varphi = 0$.

Remark 3.8. Let us stress that the resulting wave functions (21)–(22) in the analysis of the electric Aharonov–Bohm effect in [30] are just asymptotic expansions of our Airy functions (3.37).

In the coordinate representation, where $H = -\mathrm{d}_\varphi^2 + \varphi$, we can easily describe properties of the system. The time derivative of the arbitrary operator $a_t \in \mathcal{A}_t$ can be expressed with the help of the Heisenberg equation of motion in the form

$$\dot{a}_t = -\mathrm{i}[a_t, H] = \mathrm{i}[a_t, \mathrm{d}_\varphi^2] - \mathrm{i}[a_t, x], \tag{3.39}$$

where the last term is zero by the smoothness axiom. Next, we compute the metric from (3.1),

$$g_t(\mathrm{d}b_t, \mathrm{d}c_t) \overset{(3.1)}{=} -\mathrm{i}[b_t, \dot{c}_t] \overset{(3.39)}{=} [b_t, [c_t, \mathrm{d}_\varphi^2]] \overset{(3.8)}{=} 2\,\mathrm{d}_\varphi b_t\,\mathrm{d}_\varphi c_t, \tag{3.40}$$

and the metric $g_t = \frac{1}{2}$ agrees with the metric from Section 3.2.1!

We can proceed with the construction of H almost up to the end. We can construct the covariant Laplacian $\Delta = -\mathrm{d}_\varphi^2$, but in the last step we do not succeed, as a global non-zero one-form $\phi = \mathrm{d}\varphi_t$ cannot have a global potential. Indeed, as $\varphi_t \notin \mathcal{A}_t$, the one-form ϕ is not exact and the assumptions of the theorem 3.2 are not completely met. Hence, no Hamiltonian with the required properties exists.

Remark 3.9. There is a certain correspondence between SQM and the Haag–Kastler axioms for quantum field theory in $0+1$-dimensions, see [16]. The main aspect is that both settings are algebraic, the spacetime is given by (sub)algebras of observables rather than by local coordinates and topology plays a prominent role in it. There is also a similarity in their positivity requirements. The main difference is that SQM is not relativistic invariant.

3.5 Postulation of the soldering form

Finally, let us note that the algebra $\mathcal{A} = \mathcal{C}_0^\infty(\mathcal{Q}) \otimes M_2(\mathbb{C})$ provides for a description of spin degrees of freedom, however fails to relate these to the space-time geometry, not providing anything like a soldering form.

However a soldering form could be easily postulated. We can proceed with introducing certain additional structures, e.g., as in [4]. For a formulation more in the spirit of Connes' axioms [7], the structures obtained in Section 4.4 would have to be utilized.

Alternatively, we can change the underlying physical principles. For relativistic formulation of quantum mechanics the soldering form comes for free from physical data. We shall study this situation in the next Chapter.

Chapter 4

Spin and soldering structures in relativistic QM

It was clear from the beginning that the new quantum mechanics should incorporate the principles of the theory of relativity. As early as in his first communication on wave mechanics from January 1926, Schrödinger mentioned by words that he had solved also a relativistic eigenvalue equation (later called Klein–Gordon equation) but he had not published it, as it gave the wrong fine structure of the hydrogen spectrum. First it seemed that Klein–Gordon equation could be a meaningful candidate for a relativistic quantum mechanical equation.[1] But soon Dirac, Heisenberg, Pauli and others raised significant objections against it and started to look for a new equation. It turned out that relativistic invariance had enforced more substantial changes in the quantum theory.

Dirac's electron theory is considered to be one of the highlights of inter-war mathematical physics. However, the historical depiction of its genesis is often distorted by taking a starry-eyed point of view of much later recollections. In Section 4.1 the idealized picture of Dirac's heroic achievements are closely inspected and history of problems with negative energies and its interpretation by hole theory is put straight. We do not want to dispraise the value of Dirac's achievements, we just show how spinose his pathway to glory was.

In Section 4.2 we recall a generalization of scalar quantum mechanics to relativistic framework proposed in [24]. Next, general discussion of a notion of soldering form is made. It is understood in rather general form as a structure that "solders" the fibres of a vector bundle to the external geometry. Three possible ways to separate "extrinsic" and "intrinsic" structures are proposed.

Finally, in Section 4.4, we examine the vacuum of free quantum field theory given by a complex structure on phase space. The vacuum gives a soldering form for internal degrees of freedom providing them thus with spatial significance and eventually allowing them to be interpreted as spinors. To show more clearly the possibilities and limitations, the example of a (discretized) torus is discussed.

4.1 Spinose pathway to glory: Dirac's electron theory 1928–1933

In many papers on Dirac's equation a starry-eyed point of view is taken from later recollections and interviews.[2] It is clear from sources that Dirac had to struggle for his relativistic theory

[1] According to Dirac late recollections, Bohr was to have been satisfied with it, cf. below. However, Klein was Bohr's assistant.

[2] Deterrent examples are A. Pais, Playing with equations, the Dirac way, In: B.N. Kursunoglu and E. P. Wigner (ed.): *Reminiscences about a great physicist: Paul Adrien Maurice Dirac* (CUP, Cambridge, 1987), 93–116, or J. Mehra and H. Rechenberg, *The Historical Development of Quantum Theory*, Vols. IV and VI/1 (Springer, 1982, 2001). Mehra and Rechenberg even believe that Dirac's recollections are "quite definite and consistent", hence, they assume it "quite reliable". Let us quote one of their determinative remarks: "In contrast to Kragh, we would not overemphasize the nonreliability of Dirac's own account," see Vol. VI/1, p. 290.

of electron. For nearly two years he has not succeeded in finding a solution to the problem of negative energies. Even after he had proposed the hole theory, he had to modify it because of severe critique. The utmost problems were clarified at the turn of 1932–1933 and Dirac won the Nobel Prize. However, his theory has won recognition of one of the highlights of inter-war mathematical physics only later.

The history of the Dirac equation is studied in a number of essays.[3] History is often distorted by uncritical quotations of recollections from 1960s and 1970s.[4] These papers are more or less describing heroic achievements of Paul Dirac, the main character.[5] If there are any inconsistencies found in his recollections, they are immediately elucidated or excused.

Kragh has indeed pointed out that "recollections of events forty years back in time are likely to contain distortions and inaccuracies," [26, p. 53], but we think that the problem is deeper. Recollections are told with some intention and deciphering of the intensions enables one to review authenticity of the information properly.

Dirac possessed an exceptional charisma, as the recollections of his colleagues are responsible for the growth of Dirac's myth.[6] It has been forming gradually, at least since World War II, but probably already since 1930s. Nowadays, Dirac is considered to be one of the most important physicists ever lived and Dirac's equation to be one of the greatest achievements of twentieth century physics, but in the studied period of time, the attitude to Dirac was quite different. The more restrained and critical contemporary remarks are, the more pompous and grandiose later comments are. The expressions like 'magic', 'dream' or 'miracle' has appeared in this connection only since 1960s.

4.1.1 Dirac's career

Dirac's childhood and boyhood was probably affected by hard-handed upbringing of his father. Psychologically sensitive analysis was given recently by Farmelo [14], who added humbly that we can not be sure about his story. It rests mainly on Dirac's later recollections and it has no support in the sources. On the other hand, it would explain not only Dirac's personality and behaviour, but also his working style.

In 1918–21 Dirac got a first-class degree in electrical engineering in Bristol, in other two years he got degree in mathematics at Bristol University and in August 1923 he next started hid PhD study in Cambridge. In contrast with Werner Heisenberg, who was only a year older,

[3] There are two comprehensive biographies, Kragh [27] concentrates on Dirac's scientific life, whereas Farmelo [14] studies more his personal and 'inner' life, it is close to be a psychological novel. Among the topical papers, H. S. Kragh, The genesis of Dirac's relativistic theory of electrons, *Archive for the History of Exact Sciences* **24** (1981), 31–67, is great at its scope and F. Wilczek, The Dirac Equation, in: H. Baer and A. Belyaev (ed.), *Proceedings of the Dirac Centennial Symposium* (Florida State University, Tallahassee, 2002), 45–74, is interesting by its point of view of state-of-the-art in the quantum theory. Many of the papers contained in Dirac's Festschrifts *Aspects of Quantum Theory* (1972) and *The Physicist's Conception of Nature* (1973) celebrating his 70th; *Reminiscences about a great physicist: Paul Adrien Maurice Dirac* (1987) planned to celebrate his 80th, but set out only posthumously; *Tributes to Paul Dirac* (1987) from Dirac Memorial Session in 1985; *Paul Dirac, the man and his work* (1998) celebrating dedication of a plaque to him in Westminster Abbey in 1995 or *Proceedings of the Dirac Centennial Symposium* (2002) are to be used with a special caution.

[4] See interviews by T. Kuhn & al. at the beginning of 1960s, *Sources for History of Quantum Physics* (American Philosophical Society, Philadelphia, 1967). Transcript of interview with Dirac is digitized in Oral histories at Niels Bohr Library & Archives: *Interview of Dr. P. A. M. Dirac by Thomas S. Kuhn on May 7, 1963* [online at http://www.aip.org/history/ohilist/4575_3.html]. However, a significant part of Dirac's later publications are recollections, cf. Dirac's bibliography in R.H. Dalitz, *The collected works of P.A.M. Dirac, 1924–1948* (CUP, Cambridge, 1995).

[5] A. Pais, Playing with equations, the Dirac way, in: B.N. Kursunoglu and E.P. Wigner (ed.): *Reminiscences about a great physicist: Paul Adrien Maurice Dirac* (CUP, Cambridge, 1987), 93–116. Pais also takes over Dirac's recollections without having examined their correctness. Already P. Forman, A Venture in Writing History, *Science* 220 (1983), 824–827, severely criticized the so-called heroic history of quantum mechanics.

[6] "These works, written by scientists who knew Dirac personally, express physicists' homage to a great colleague," H. S. Kragh, *Dirac – A Scientific Biography* (CUP, Cambridge, 1990), p. ix.

he did not prove his brilliance within his studies: "His contributions were interesting, but not remarkably so, and not of striking originality," [27, p. 12]. But his self-confidence was growing and his time was only to come. In 1925 he studied his final year in Cambridge, he was at the right time in the right place.

After graduation in June 1926 Dirac spent a year on the Continent, in Copenhagen with Niels Bohr and in Göttingen with Max Born and Werner Heisenberg. After having returned to Cambridge in November 1927, he was elected a Fellow of St. John's College. His scientific reputation was rapidly growing. After all, the formulation of the relativistic equation for one electron at the turn of 1927–28 brought fame to him.[7] In 1930 he wrote one of the most influential books on Quantum Mechanics, *The Principles of Quantum Mechanics* [10] and he was elected a Fellow of Royal Society of London (in his 28 years). In 1932 he took the Lucasian Chair of Mathematics at Cambridge University. In the next year 1933 he won the Nobel Prize.

4.1.2 Relativistic quantum theory of the electron

In 1926 the first attempts for a relativistic version of quantum mechanics (more precisely Schrödinger's wave mechanics) appeared. Schrödinger's eigenvalue equation for a free electron

$$E\psi = H\psi, \tag{4.1}$$

with $H = \boldsymbol{p}^2/2m$ a non-relativistic kinetic energy, is not Lorentz invariant. After transition from classical to quantum mechanics accomplished by

$$E \longrightarrow \mathrm{i}\hbar\frac{\partial}{\partial t}, \qquad \boldsymbol{p} \longrightarrow -\mathrm{i}\hbar\nabla, \tag{4.2}$$

it gives a differential equation of the first order in time derivative and of the second order in spatial derivatives:

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi. \tag{4.3}$$

Nevertheless, the theory of relativity demands an equal footing for space and time.

One attempt, carried out first by Oskar Klein, utilized the classical relativistic expression for the energy

$$E^2 = p^2c^2 + m^2c^4 \tag{4.4}$$

and set $H = +\sqrt{p^2c^2 + m^2c^4}$ into the Schrödinger equation (4.1). The result is

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = c\sqrt{p_1^2 + p_2^2 + p_3^2 + m^2c^2}\,\psi. \tag{4.5}$$

It is possible to expand the square-root operator in an infinite series of derivative operators, but there was little faith in such a process. However, at least for some time, Pauli seriously considered this equation.[8]

As in Fourier expansion of H derivatives of any order appeared, the problem of unsymmetrical time and space derivatives remained. Moreover, Klein found it impossible to include external fields in relativistically invariant way. So, he decided to get rid of the square root by squaring

[7] He published his first important results (introducing Poisson brackets to QM, perturbation theory and so-called Fermi–Dirac statistics) only a month after his rivals (Born–Jordan–Heisenberg, Heisenberg and Fermi). This is thoroughly discussed by Kragh [27]. I believe it is one of the reasons of his withdrawnness. After it all, he longed for a break-through even more.

[8] Despite its unpleasant form, Pauli regarded it as in itself sensible and preferred it to (4.6): "Herr Pauli regards the relativistic wave equation of second order with much suspicion," Kudar to Dirac, December 21, 1926, quoted according to [27, p. 54].

the whole equation,[9] or (which turns to be the same) using directly the relativistic expression for the energy (4.4) in quantization procedure (4.3) and got the equation

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = (-\hbar^2 \nabla^2 c^2 + m^2 c^4)\psi. \tag{4.6}$$

This equation was independently obtained by several other physicists and now it is known under the name Klein–Gordon equation.[10] Its 4-dimensional form allowed to define a 4-vector of charge and a current densities satisfying the continuity equation. Nevertheless, as already mentioned, it did not give the correct fine structure of the hydrogen spectrum.

The other 'heuristic' approach, based on ideas of W. Pauli, was carried out by Jordan and Heisenberg in spring 1926. They tried to include relativistic effects as perturbations. So, they derived the first approximation to the fine structure formula and added a term referring to the electron spin. "Despite of its empirical success, the theory was not genuinely relativistic and could not explain the described phenomena," cf. [27, p. 52].

Motivations: Dirac's attitude to the Klein–Gordon equation

There are different opinions on Dirac's exact intention. Was he trying to get the simplest possible relativistic quantum theory? Or was he trying to derive a relativistic description of the spin? Dirac himself expressed his intention several times, but particular versions are inconsistent.

In November 1926, Dirac seems to have considered the Klein–Gordon theory as a serious candidate for a relativistic quantum mechanics, however, only for a short time. He even thought about Klein's idea of a 5-dimensional theory embracing both quantum mechanics and general relativity for some time.[11] But he soon abandoned those ideas. The main objection probably was that the Klein–Gordon equation was not an evolution equation. The second derivatives with respect to time did not allow a proper quantum mechanical interpretation; it was in variance with the general transformation theory of him and Jordan.

Dirac liked to tell a story about Bohr asking him "what are you working on now?" Dirac replied that he was trying to get a satisfactory relativistic theory of the electron. Then Bohr said, "But Klein and Gordon have already solved that problem." In the next part of the story Dirac's recollections seriously contrast:

> 1963: "I remember it disturbed me quite a lot that Bohr was so satisfied with it because of the negative probabilities that it led to."[12]
>
> 1974: "I was quite taken aback. It rather surprised me that such an emminent physicist as Bohr should be satisfied with the Klein–Gordon equation and I started to explain why I was not satisfied with it. But just then the lecture started and I was never able to finish it."[13]
>
> 1977: "I didn't have time to explain my objections fully to Bohr on that occasion, but I could see where his opinions lay, and that was the opinion of most physicists

[9] It is allowed to square the eigenvalue equation $A\psi = B\psi$ if $[A, B] = 0$.

[10] It was first obtained by Schrödinger but remained unpublished. In spring 1926 it was first published by Oskar Klein. Then, during 1926, it was thoroughly studied by L. de Broglie, V. Fock, W. Gordon, E. Schrödinger, J. Kudar and others. See H. Kragh, Equation with many fathers: the Klein–Gordon equation in 1926, *American Journal of Physics* 52 (1984) 1024–1033.

[11] [27, p. 53], according to a letter from Heisenberg to Pauli, November 4, 1926 [19, Vol. I, p. 352].

[12] *Interview of Dr. P.A.M. Dirac by Thomas S. Kuhn on May 7, 1963*, Niels Bohr Library & Archives, American Institute of Physics, College Park, MD USA, [online at http://www.aip.org/history/ohilist/4575_3.html]. However, it was shown by Kragh that the problem of the negative probabilities appeared much later, see H. S. Kragh, The genesis of Dirac's relativistic theory of electrons, *Archive for the History of Exact Sciences* **24** (1981), p. 64.

[13] P.A.M. Dirac, An historical perspective on spin, in: J.B. Roberts (ed.), *Proc. Summer Studies of High-Energy Physics with Polarized Beams*, July 22–26, 1974 (Argonne National Laboratory, Argonne, 1975). Rep. ANL/HEP 75-02, p. XXXII–8.

> of that time, perhaps all of them."[14]
>
> 1975/78: "It rather opened my eyes to the fact that so many physicists were quite complacent with a theory which involved a radical departure from the basic laws of QM, and they did not feel the necessity of keeping to these basic laws in the way that I felt."[15]

This is one of the Dirac's late stories. As we do not know Bohr's opinion on the Klein–Gordon theory from independent sources, we have to ask what the story tells us. All these facets indicate that it was told with the only aim: to show Dirac as a visionary who foresees the progress in quantum mechanics better than Bohr, the leader of the community himself!

Kragh accepted that the story is true, even though he admitted that "Dirac's accounts of the event are not entirely consistent." My opinion is that Dirac wanted to get a relativistic equation for a quantum particle. The incorporation of the spin was a secondary aim, which was added later in the course of solving proposed conditions.

This hypothesis would also explain why Dirac succeeded. He proceeded indirectly (regardless if consciously or unconsciously). He derived his equation from basic principles of quantum mechanics and special relativity theory. It was a product of mathematical reasoning, he would have never introduced it with an empiricist approach: "Dirac's success in finding the accurate equation shows the great superiority of principle over the empirical method."[16] Several eminent physicists, namely Wolfgang Pauli in Zürich, Eugene Wigner and Pascual Jordan in Göttingen, C.G. Darwin in Cambridge, Hendrik Kramers in Utrecht, Yakov Frenkel, Dimitri Iwanenko and Lev Landau in Leningrad tried to proceed empirically and simply construct a pair of equations to represent the fine structure of the hydrogen spectrum, see [27, p. 59–60].

Linearization of the relativistic energy expression

> "Our problem is to obtain a wave equation of the form $(H - E)\psi = 0$, which shall be invariant under a Lorentz transformation and shall be equivalent to (1) [Klein–Gordon equation] in the limit of large quantum numbers."
>
> P.A.M. Dirac [8, p. 613]

Dirac finished his paper *The Quantum Theory of the Electron* [8] after a year of concentrated efforts during Christmas 1927. It was published within three weeks of January 1928, in a great haste, as Dirac feared to be outrun again (cf. footnote 7). It is probably Dirac's best paper. Surely it is the most famous one.

Dirac started with the same equation (4.5) as Klein, but before putting it into the Schrödinger equation, he argued that "the symmetry between p_0 and p_1, p_2, p_3 required by relativity shows that, since the Hamiltonian we want is linear in p_0, it must also be linear in p_1, p_2, p_3." So, he tried to express the sum of the squares as a square of some modified terms, which would transform it into a linear form

$$(p_0 + \alpha_1 p_1 + \alpha_1 p_1 + \alpha_1 p_3 + \beta)\psi = 0, \tag{4.7}$$

[14] P.A.M. Dirac, The Relativistic electron Wave Equation, Proc. European Conf. on Particle Physics, Budapest, Hungary, July 4–9, 1977, Preprint KFKI-1977-62, p. 10. However, Dirac knew very well that other physicists were also trying to improve or supersede the Klein–Gordon equation. e.g., Pauli (cf. footnote 8). Also Heisenberg recognized the significance of linearity in Schrödinger's equation and considered equations of the Klein–Gordon type to be without prospect, cf. W. Heisenberg, Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik, *Zeitschrift für Physik* 43 (1927), p. 184.

[15] P.A.M. Dirac, *Directions in Physics: lectures delivered during a visit to Australia and New Zealand, August/September 1975.* (Wiley, New York, 1978), p. 15.

[16] C.G. Darwin, The wave equation of the electron, *Proceedings of the Royal Society of London. Series A, Mathematical and Physical*, Vol. 118 (1928), p. 664.

Multiplying with the conjugate equation, comparing with the Klein–Gordon equation (4.6) and setting $\beta = \alpha_4 mc$ gave him the conditions

$$\alpha_\mu^2 = 1, \qquad \alpha_\mu\alpha_\nu + \alpha_\nu\alpha_\mu = 0\ (\mu \neq \nu), \qquad \mu, \nu = 1, 2, 3, 4, \tag{4.8}$$

which are similar to propreties of Pauli spin matrices. However, there are just three of them in $M_2(\mathbb{C})$,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Then he got another smart idea, he proposed αs to be 4×4 matrices and he used Pauli matrices to construct them: he first defined[17]

$$\sigma_i' = \begin{pmatrix} \sigma_i & \mathbf{0} \\ \mathbf{0} & \sigma_i \end{pmatrix}, \qquad \rho_1 = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix}, \qquad \rho_2 = \mathrm{i}\begin{pmatrix} \mathbf{0} & -\mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix}, \qquad \rho_3 = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}, \tag{4.9}$$

and then he got[18]

$$\begin{aligned} \alpha_1 &= \rho_1\sigma_1' = \begin{pmatrix} \mathbf{0} & \sigma_1 \\ \sigma_1 & \mathbf{0} \end{pmatrix}, \qquad \alpha_2 = \rho_1\sigma_2' = \begin{pmatrix} \mathbf{0} & \sigma_2 \\ \sigma_2 & \mathbf{0} \end{pmatrix}, \\ \alpha_3 &= \rho_1\sigma_3' = \begin{pmatrix} \mathbf{0} & \sigma_3 \\ \sigma_3 & \mathbf{0} \end{pmatrix}, \qquad \alpha_4 = \rho_3 = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}. \end{aligned} \tag{4.10}$$

This is usually called the Dirac representation of α-matrices, as the solution of the conditions (4.8) is not unique. Other important solutions are due to Majorana and Weyl, confront, e.g., Thaller [39, p. 36].

The wave equation (4.7) takes the form

$$(p_0 + \rho_1\boldsymbol{\sigma}\cdot\boldsymbol{p} + \rho_3 mc)\psi = 0 \tag{4.11}$$

and it is called Dirac equation.

Features of the Dirac equation

At this stage, Dirac's equation was only an inspired guess [27, p. 60]. But more detailed analysis immediately followed. The next step was a proof that the Dirac equation is Lorentz covariant. Namely, in the form of (4.11) Lorentz covariance is not manifest. Putting $\gamma_r = \rho_2\sigma_r'$ and $\gamma_4 = \rho_3$, Dirac introduced a different representation of his matrices, later called *Dirac γ-matrices* and transformed his equation into the manifestly covariant form

$$\Big(\mathrm{i}\sum_{\mu=1}^{4}\gamma_\mu p_\mu + mc\Big)\psi = 0, \tag{4.12}$$

with $p_0 = \mathrm{i}\,p_4$. Proving the correct transformation properties of γ_μ yields Lorentz covariance, see [8, p. 615–617].

Subsequently, Dirac studied an electron in an arbitrary electromagnetic field with a scalar and vector potential A_0 and $\boldsymbol{A}$, respectively. Substituting

$$p_0 \longrightarrow p_0 + \frac{e}{c}A_0, \qquad \boldsymbol{p} \longrightarrow \boldsymbol{p} + \frac{e}{c}\boldsymbol{A},$$

[17] We are forced to denote the four-dimensional Pauli matrices with a prime, σ_i', while Dirac denotes them with the same symbol σ_i as the original Pauli matrices. We also denote by $\mathbf{0}$ and $\mathbf{1}$ zero and unit 2×2 matrices respectively.

[18] Kragh [27, p. 60] mixes up the role of ρs, σs and αs.

he got a Hamiltonian which differs from the previous relativity Hamiltonian of Klein and Gordon by the following two extra terms

$$\frac{e}{c}\boldsymbol{\sigma}\cdot(\nabla\times\boldsymbol{A}) \qquad \text{and} \qquad \mathrm{i}\,\frac{e}{c}\rho_1\boldsymbol{\sigma}\cdot(\nabla A_0).$$

The second term is argued not to be observable, as it is pure imaginary.[19] The first term gives exactly the value for the magnetic moment assumed in the spin electron model. Thus, spin is deduced from the principles of relativistic quantum mechanics. Hence, the Dirac equation is capable to explain (in first approximation) the correct doublet splitting of hydrogen terms.[20] W. Gordon and C.G. Darwin proved quickly that the Dirac equation reproduces exactly the fine structure of the hydrogen atom.

It was a great success. Yet, Dirac embellished the story in 1970s by insisting on the fact that he was not interested in explaining the spin and that he did not make use of Pauli's work. He even claimed that he discovered Pauli matrices by himself, independently of Pauli.[21] This exaggeration was noticed by Kragh, but excused by asserting that the use of spin matrices was "heuristic only" [27, p. 60]

Still, one problem of the initial Klein–Gordon equation remained unsolved. Every solution of the equation gives rise to another solution with negative energy. Dirac knew about this problem from the beginning: "One gets over the difficulty on the classical theory by arbitrarily excluding those solutions that have a negative [energy] W. One cannot do this on the quantum theory, . . . " [8, p. 612]. In comparison with success of his theory Dirac did not first considered the problem of negative energies so compelling.[22]

Reception of Dirac's theory: prompt appreciation and subsequent animadversion

In the preserved correspondence, we mostly find a positive reception of Dirac's paper.[23] However, later recollections have more panegyric features. In 1928 a simple collegial appreciation was expressed, whereas since 1960s it has rather been a homage to the hero of the quantum generation.[24] Dirac depreciated his success in the 1960s claiming that he found out the solution "by playing around with mathematics." However, Pais took the claim seriously and considered it for Dirac's general way of doing research.

However, in summer 1928 the attitude to Dirac's theory changed. In June 1928 Dirac was invited by Heisenberg to give lectures on his theory in Leipzig. Heisenberg was disappointed that Dirac had not been able to address the problem of negative energies.[25] Dirac worked on the problem, but without any success.

[19] In 1935 Andrew Lees (a student of Dirac) has shown that the electric moment does not appear in fact, A. Lees, The electric moment of an electron, *Proceedings of the Cambridge Philosophical Society* 31 (1935) 94–97;

[20] Later, Dirac insisted on the assertion that he did not attempt to obtain exact solution, because he was afraid that the higher order corrections would not come out right. Kragh did not believe it and ascribes it to the haste in publication motivated by competition and fear of not being the first to publish the idea. "After all, if it had the crucial importance for Dirac, he would have attempted the exact fine structure formula later, but he did not," see [27, p. 61–62].

[21] P.A.M. Dirac, Recollections of an exciting era, in: C. Weiner (ed.), *History of Twentieth Century Physics* (Academic Press, New York, 1977) p. 139.

[22] "The resulting theory is therefore still only an approximation, but it appears to be good enough" [8, p. 612].

[23] "Dirac has got a new system of wave equations which does the whole spinning electron correctly, Thomas correction, relativity and all," Darwin to Pauli, January 11, 1928, [19, Vol. I, p. 424]; "I admire your last work about the spin in the highest degree," Heisenberg to Dirac, February 13, 1928, quoted according to [27, p. 62].

[24] E.g., Dirac's derivation of spin "was regarded as a miracle. [. . .] It was regarded really as an absolute wonder," Oral histories at Niels Bohr Library & Archives: *Interview of Dr. Leon Rosenfeld by T. S. Kuhn and J. L. Heilbron at Carlsberg on July 1, 1963* [online at http://www.aip.org/history/ohilist/4847_1.html].

[25] "I am much more unhappy about the question of the relativistic formulation and about the inconsistency of the Dirac theory. Dirac was here and gave a very fine lecture about his ingenious theory. But he has no more of an idea than we do about how to get rid of the difficulty $e \longrightarrow -e$," Heisenberg to Bohr, June 23, 1928, quoted according to [27, p. 66].

At the end of 1928, the situation got even worse. Oscar Klein proved that for a very simple case of an electron scattering from a potential barrier with sufficient energy Dirac's theory gives absurd results. Instead of observed electron tunnelling into a barrier with exponential damping, the theory predicted that electron would be always transmitted. The result became known as Klein paradox.[26]

4.1.3 Hole theory

The problem of negative energy solutions of Dirac's equation was a peculiar one. Dirac was bothered by the problem for a very long time. It is usually not stressed that it took him nearly two years until he came with an attempt at a solution in December 1929. However, Dirac did not solve it mathematically. He indicated the problem as interpretational and claimed that "... all the states of negative energy are occupied except perhaps a few of small velocity. [...] Only the small departures from exact uniformity, brought about by some of the negative-energy states being unoccupied, can we hope to observe. The holes in the distribution of negative-energy electrons are the protons," [9, § 2]. On six pages of the paper, there are only four equations.

It is clear that this is a fall-back solution. However, Dirac explained it with the help of the exclusion principle, a famous theory by Wolfang Pauli, his greatest opponent and critic.[27]

Dirac stressed the philosophically appealing aspects of the theory: "We require to postulate only one fundamental kind of particle, [...]. The mere tendency of all the particles to go into their states of lowest energy results in all the distinctive things in nature having positive energy," [9, p. 363–364]. On the other hand, the hole theory did not explain dissymmetry between electrons and protons, in particular their different masses.

Reactions to the hole theory were rather sceptical.[28] Unofficially it was considered to be pure nonsense.[29] Moreover, Heisenberg and Pauli soon proved that the holes must possess the same mass as the electron. When Tamm and Oppenheimer computed the lifetime of electrons and protons according to the hole theory, they got absurd results: 10^{-3} s for proton and 10^{-9} s for electron. Treating an electron hole as a proton was not sustainable anymore.

In summer 1931 Dirac had to rethink the concept of holes. When he had eliminated the impossible, there remained merely one unpleasant and improbable possibility. Dirac followed the logic of Sherlock Holmes and (unwillingly) concluded that each hole corresponded to "a new kind of particle unknown to experimental physics, having the same mass and opposite charge to an electron,"[30] Thus, Dirac was compelled to propose new (anti) particles, anti-electron and also anti-proton.

In autumn 1932, the discovery of the positron by Anderson in USA and its confirmation by Blackett and Occhialini directly in Cambridge retrospectively proved justness of Dirac's hypothesis. Yet, Dirac hesitated to identify his anti-electron with Anderson's positron. Bohr,

[26] "Dies dürfte als ein besonders schroffes Beispiel der von Dirac hervorgehobenen Schwierigkeit der relativistischen Dynamik zu betrachten sein." O. Klein, Die Reflexion von Elektronen an einem Potentialsprung nach der relativistischen Dynamik von Dirac, *Zeitschrift für Physik* 53 (1929), 157–165.

[27] Pauli first appreciated the theory, admittedly merely on account of an intermediated information, "Was ich höre klingt hoffnungsvoll," Pauli to Jordan, November 30, 1929, [19, Vol. I, p. 526]. After getting thoroughly acquainted with Dirac's work, he reppraised his opinion, "Ich glaube jetzt *gar nicht mehr* daran!" Pauli to Klein, February 10, 1930, [19, Vol. II, p. 4], the emphasis is due to Pauli. Animosity between Dirac and Pauli seems to be enhanced in the description of Kragh [27, p. 112–114]. Farmelo [14] even gave to Pauli the role of the main villain and Dirac's archenemy. He also used the animosity as a leitmotiv in a couple of stories from Dirac's life.

[28] Heisenberg wrote to Dirac: "it is certainly a great progress. [...But] I cannot see yet, how the ratio of the masses etc. will come out," December 7, 1930. In a letter to Bohr, Heisenberg expressed his sceptical opinion more unreservedly (a letter from December 20, 1929).

[29] Apart from Fermi and Pauli, e.g., Lev Landau commented Dirac's lecture on the hole theory — delivered at British Association for the Advancement in Science Congress in Bristol — with a single word "Quatsch" translated as "rubbish" in [14] and as "nonsense" in [27].

[30] [11, p. 61]. The metaphor with Sherlock Holmes is due to Farmelo [14].

Heisenberg and Pauli were also not convinced.[31] Opposition to the hole theory was getting weaker slowly, but it was gradually vindicated.[32]

Contrary to the opinion frequently repeated in literature, the discovery of the positron was not a consequence of the theoretical prediction made by Dirac. It was made independently and, moreover, it took some time until it was generally accepted that Dirac's anti-electron and Anderson's positron are the same thing.

4.1.4 Nobel Prize

At the end of 1933 the decision on the Nobel Prize for 1932 and 1933 should be made. Although the report, prepared for the Nobel Prize Committee of the Royal Swedish Academy by Carl Wilhelm Oseen, was very critical in comparison to the present evaluation of Dirac's work[33] and although Dirac obtained only two nominations,[34] on the recommendation of the Committee Academy decided to give the Prize for 1933 to Heisenberg and to divide the Prize for 1933 between Schrödinger and Dirac, who became the youngest theorist to have received the Nobel Prize.

Oseen also writes in the report that Dirac could obtain his best results only in the future. Dirac later published many important results in other physical disciplines. However, he did not carry out the seemingly achievable refinement of his theory and some interpretational problems have remained open.[35] Dirac later opposed to the development in QED. In particular, he did not agree with renormalization theory (1948), and he left the mainstream of theoretical physics. Still, his fame was growing and his ideas were gradually accepted.

We have shown that the value of Dirac's ideas became appreciated only later. It would be inaccurate to believe in the starry-eyed point of view of recollections from that later time describing a harmonic development of science.

4.2 Spectral relativistic quantum mechanics

Relativistic invariance enforces substantial changes in the framework of non-relativistic quantum theory. Let us modify the notion of scalar quantum mechanics introduced in Section 3.1 to agree with requirements of special theory of relativity. From the spectral point of view, we would like to have the following requirements fulfilled, see Kopf and Paschke 2005 [24]:

(a) Order one condition: In contrast to the smoothness requirement of the non-relativistic SQM, the time evolution satisfies

$$\mathrm{i}[\mathcal{A}_t, \dot{\mathcal{A}}_t] = 0, \qquad \forall t \in \mathbb{R},$$

cf. Section 3.3.2. Hence, the Hamiltonian generating the time evolution is at the most of first order and uncertainty relations seem to be dropped.

(b) Stability of the vacuum: A vacuum state is determined by a complex structure J on the Hilbert space $\mathcal{H}$ and it commutes with the Hamiltonian,

$$[H, J] = 0.$$

[31] "I do not believe on your perception of 'holes', even if the existence of the 'antielectron' is proved." Pauli to Dirac, May 1, 1933, [19, Vol. II, p. 159].

[32] Pauli suppressed his critique by the end of June 1933: "ich bin also nicht abgeneigt, an eine Art reformierte Löchertheorie zu glauben," Pauli to Heisenberg, July 14, 1933, [19, Vol. II, p. 187].

[33] "[Dirac's] work is not fundamental in the same sense as Heisenberg's. [...] He is independent... but a successor in relation to Heisenberg. If one asks if Dirac is a scientific pioneer of the same dimension as Planck, Einstein or Bohr, the answer must for the present be, I think, definite no. [...] so far it has not left him the time for really great innovative work... It is noteworthy that Dirac's most original papers stem from the last years," Nobel archive, cited according to [27, p. 115–116].

[34] Schrödinger obtained 11 nominations (i.a. from Bohr and Einstein). The other physicists nominated for the Prize: Sommerfeld, Bridgman, Davisson and Paschen obtained more nominations than Dirac, see [27, p. 116].

[35] Very nice and modern account of the problems related to the interpretation of the Dirac equation was given by Thaller in the first chapter of his book [39].

However, in accordance with our aim to construct a one-particle theory, this condition may not be satisfied if particles are produced due to external fields or spacetime curvature.

(c) Physical states: Eigenspace projections $P_\pm$ of J coincide on static spacetimes with the projections on positive and negative frequencies. In order to ensure suitable spectral properties of the Hamiltonian, only one of the two eigenspaces of J, the space of positive energy solutions is considered. Hence, the physical states of the Hilbert space are given by the range of the eigenspace projection P_+ of the complex structure J. Physical observables a_{phys} have to preserve the space of physical states, i.e.

$$[a_{\text{phys}}, J] = 0.$$

Elements a of the algebras $\mathcal{A}$ describing the space geometry fail to be observables. This may be remedied by their restriction to the eigenspaces of J, obtaining thus physical observables a_{phys}:

$$a_{\text{phys}} = P_+ a P_+ + P_- a P_- \qquad \text{for all } a \in \mathcal{A}.$$

However, starting with a commutative algebra $\mathcal{A}$, its physical counterpart $\mathcal{A}_{\text{phys}}$ may no more commute! Thus uncertainty, lost in its replacement through the order-one condition (a) creeps in through a back door.

We do not employ the possibility to construct a set of commuting and at the same time physical observables, as determined by the Newton–Wigner states, and keep the directly received noncommutative observables, which were already obtained in a remarkable paper by M.H.L. Pryce in 1948, see [35].

The above requirements give a set of structures necessary for the formulation of the theory, but they do not fix it entirely. This freedom can be restricted to a large degree by postulating symmetries.

On an example of a free spinor field on Minkowski spacetime it was argued that physical observables x_{phys} corresponding to the spatial coordinates x_i indeed fail to commute:

$$[x_{i,\text{phys}}, x_{j,\text{phys}}] = \mathrm{i}\epsilon_{ijk} S_k,$$

where S_k is the spin vector, see [24]. The latter equation provides us with a structure that "solders" coordinates on the configuration manifold with spin coordinates. We devote us to more thorough discussion of this notion in the next Section.

4.3 Soldering structures

In classical geometry, a vector bundle without any additional structure represents in its fibres purely internal degrees of freedom, with no reference to the external geometry of the space. Spinor bundles are not of this kind: the spinor bundle is a vector bundle but related to the external geometry represented by the tangent bundle through a soldering form. The soldering form "solders" the fibres of the spinor bundle to the external geometry.

Let us consider a fibered manifold $\pi : E \longrightarrow \mathcal{Q}$. Local coordinates on a configuration manifold $\mathcal{Q}$ of a physical system are often referred to as the extrinsic (external) degrees of freedom. On the contrary, the fibered coordinates on E projected to $\mathcal{Q}$ are usually referred to as intrinsic (internal) coordinates.

However, taking the soldering form conceptually as a special structure relating intrinsic degrees of freedom locally to extrinsic ones, a generalization to more general, noncommutative spaces may be attempted. This depends decisively on the meaning of "extrinsic" and "intrinsic". Therefore, a definition of a soldering structure will depend on a chosen context and no general and mandatory definition of soldering form is to be expected. Let us discuss certain possible notions used to distinguish the extrinsic and intrinsic structures.

The first possibility is to distinguish the extrinsic and intrinsic structures with the help of the algebra of coordinates $\mathcal{A}$ represented on a suitable Hilbert space $\mathcal{H}$. If $[X, \mathcal{A}] = 0$ then X is intrinsic, otherwise it is extrinsic. A typical extrinsic operator is angular momentum L. On the other hand, the spin operators S are intrinsic.

The second possibility is to base the notions of extrinsic and intrinsic structures on the action of automorphisms of the algebra of coordinates of a space given by a spectral triple $(\mathcal{A}, D, \mathcal{H})$, see e.g. [7].

An automorphism of algebra $\mathcal{A}$ is a mapping $\phi : \mathcal{A} \longrightarrow \mathcal{A}$ which preserves the algebraic structure of $\mathcal{A}$, i.e.,

(i) ϕ is linear, $\phi(\lambda a + b) = \lambda\phi(a) + \phi(b)$,

(ii) ϕ preserves multiplication, $\phi(ab) = \phi(a)\phi(b)$,

(iii) ϕ respects the $*$-operation, $\phi(a^*) = \phi(a)^*$.

An automorphism acts on intrinsic degrees of freedom only, if it is so-called inner automorphism. Then it is generated by a unitary in the algebra $\mathcal{A}$, i.e., it is of the form $\alpha_u(\phi) = u^*\phi u$, with $\phi \in \mathcal{A}$ and u unitary. The group $\mathrm{Int}(\mathcal{A}) \subset \mathrm{Aut}(\mathcal{A})$ of inner automorphisms is a normal subgroup that describes intrinsic gauge transformations.

If ϕ is inner automorphism of a commutative algebra $\mathcal{A}$, then the condition $\phi(a) = u^*au$ gives $u(x) = \mathrm{e}^{\mathrm{i}\phi(x)}$, $\phi(x) \in \mathbb{R}$. As $\mathcal{A}$ is commutative, $u^*au = \mathrm{e}^{-i\phi(x)}\, a\, \mathrm{e}^{i\phi(x)} = a$ and ϕ is just identity.[36]

On the other hand, as noted in [7], for highly noncommutative spaces all automorphisms may turn out to be intrinsic. In that case one would thus expect the concept of a soldering form to become void of content.

The third possibility is based fundamentally on the unbounded selfadjoint operator D of spectral geometry, more precisely on its spectral decomposition. This decompostion is not unique and should not be expected to be.[37] If the structures of the decomposition do not fully capture the nature of D, there remain then degrees of freedom intrinsic to the geometry of the decomposition which can be soldered to the extrinsic geometry through the remaining information in D thus giving rise to a soldering form. The implementation of this structures by means of rising operators of transporters p, developed in Section 2.2, is currently in progress. However, it is already clear that we can sort out the intrinsic degrees of freedom from the extrinsic ones by means of the rising operators u of the transporters p: If $[X, u] = 0$, then X is intrinsic. Otherwise it is extrinsic.

It should be noted that some choices in the setup of the taken path seem to be in some cases not strictly necessary and in other cases perhaps not the most general ones. Thus the setup should not be considered to be in its most useful and definitive form and should be rather understood as open to further improvement. We investigate the first possibility in the next Section.

4.4 Positive energy projectors and spinors

The vacuum of free quantum field theory is determined by a complex structure J on the one-particle complex Hilbert space $\mathcal{H}$, the classical phase space. It is shown here that such a structure can supply a represented algebra $\mathcal{A}$ with a soldering form that relates internal degrees of freedom, i.e., the eigenspaces of $\mathcal{A}$ in $\mathcal{H}$ with geometric structure. In this way, the standard soldering form of spin geometry can be recovered.

A case of particular interest is the torus since its spin structure was recently discussed not only in the classical but also in the noncommutative case [34] in the setting of A. Connes' axioms [7] for spectral geometry. Connes' axioms provide automatically for a spin structure and capture

[36] For $\mathcal{A} = C^\infty(\mathbb{T}^n) \otimes M_p(\mathbb{C})$ are the inner automorphisms gauge transformations, e.g. $\mathrm{e}^{i\phi(x)} \otimes a_{i_1 \cdots i_p}$.

[37] Cf. M. Kac, Can one hear the shape of a drum? *American Mathematical Monthly* **73** (1966)(No. 4, part 2), 1–23; J. Milnor, Eigenvalues of the Laplace operator on certain manifolds, *Proc. Nat. Acad. Sci.* **51** (1964) (4), 542; T. Sunada, Riemannian coverings and isospectral manifolds, *Annals of Mathematics* **121** (1985), 169–186.

well much of the essentials of geometry. The here presented approach is not intended to achieve the same degree of completeness but rather to provide an alternative, physically motivated point of view on structures that may be eventually obtained otherwise.

The example illustrating the chosen approach in this work is the discretized torus $\mathbb{T}_{(n_1,n_2)}$. Its particularities are spelled out in Section 4.4.1 in order to fix the notation. Section 4.4.2 discusses invariant vacua given by invariant complex structures and determines their high-frequency behavior. The soldering form is obtained in Section 4.4.3. Corresponding facts on continuous tori are mentioned throughout for comparison. The significance of the presented approach is discussed in the Conclusion.

Given the physical motivation of the taken approach, it is interesting to compare the results with the situation of an ordinary spin structure, understood as the phase space (space of initial conditions) of a Dirac field on a corresponding $2+1$-dimensional flat spacetime. Such a comparison justifies the interpretation of the high energy limit of the complex structure as the soldering form. This is worked out in the Appendix, after a short review of basic facts on spin structures over low-dimensional Minkowski space. It is also shown there for completeness that while the spin rotation matrix (which would also qualify for a soldering structure) is generally visible in the commutator of the physical coordinates x^i_P, this is not applicable in our case as the commutator vanishes in the high energy limit in two dimensions.

4.4.1 Preliminaries

The discretized torus $\mathbb{T}_{(n_1,n_2)}$ is the space of the group $G = \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2}$. The group G acts on $\mathbb{T}_{(n_1,n_2)}$ by translations and is the counterpart of the symmetry $U(1) \times U(1)$ of the ordinary (undiscretized) torus $\mathbb{T}^2$.

In particular, the action of $g = [g_1, g_2] \in G$ on point $x = [x_1, x_2] \in \mathbb{T}_{(n_1,n_2)}$ is given by:

$$g(x) = [g_1, g_2]([x_1, x_2]) = [g_1 + x_1 \mod n_1, g_2 + x_2 \mod n_2] \tag{4.13}$$

and in the generators $V_1 = (1, 0)$ and $V_2 = (0, 1)$ of G act by

$$\begin{aligned} V_1(x) &= [1, 0]([x_1, x_2]) = [x_1 + 1 \mod n_1, x_2] \\ V_2(x) &= [0, 1]([x_1, x_2]) = [x_1, x_2 + 1 \mod n_2] \end{aligned} \tag{4.14}$$

The geometry of the discretized torus $\mathbb{T}_{(n_1,n_2)}$ consists of $n_1 n_2$ points and can be described via the Gel'fand transform by an $n_1 n_2$-dimensional commutative C^*-algebra $\mathcal{A} = C(\mathbb{T}_{(n_1,n_2)}, \mathbb{C})$ of complex functions on $\mathbb{T}_{(n_1,n_2)}$. The action of $\mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2}$ on $\mathbb{T}_{(n_1,n_2)}$ induces a corresponding action on the C^*-algebra $\mathcal{A}$:

$$g(a)(x) = a(g(x)) \qquad \text{for all } g \in G,\ a \in \mathcal{A} \text{ and } x \in \mathbb{T}_{(n_1,n_2)} \tag{4.15}$$

To simplify calculations, the same notation will be used for the algebra $\mathcal{A}$ and its representation on $\mathcal{H}$. In addition, it will be assumed that the action of the symmetry group G is unitarily implemented on $\mathcal{H}$ and the same notation will be used for the group and its unitary representation.

In order to fix $\mathcal{H}$ and at the same time to allow for intrinsic degrees of freedom to be later interpreted as spin, we choose $\mathcal{H} = L^2(\mathbb{T}_{(n_1,n_2)}) \otimes \mathbb{C}^2$, where $L^2(\mathbb{T}_{(n_1,n_2)})$ is the up to unitary equivalence unique representation space of the smallest faithful involutive representation of $\mathcal{A}$ with the obvious unitary implementation of the symmetry group G:

$$g(\phi)(x) = \phi(g(x)) \qquad \text{for all } g \in G, \phi \in L^2(\mathbb{T}_{(n_1,n_2)}) \text{ and } x \in \mathbb{T}_{(n_1,n_2)}, \tag{4.16}$$

to be extended trivially to $\mathcal{H}$:

$$g(\phi \otimes v)(x) = \phi(g(x)) \otimes v \tag{4.17}$$

for all $g \in G, \phi \in L^2(\mathbb{T}_{(n_1,n_2)}), v \in \mathbb{C}^2$ and $x \in \mathbb{T}_{(n_1,n_2)}$.

More generally, one may take $\mathcal{H} = L^2(\mathbb{T}_{(n_1,n_2)}, \mathbb{C}^2)$, i.e., the square integrable sections of a fibre bundle with base space $\mathbb{T}_{(n_1,n_2)}$ and fibre $\mathbb{C}^2$. The above choice corresponds to the fibre bundle being trivial. This is of course not a topological statement as the discretized torus carries the discrete topology but rather a statement on the action of the symmetry group G. Nontrivial actions could be obtained introducing a sign in (4.17):

$$g(\phi)(x) = (-1)^{s_1((g_1+x_1)/n_1)^\star + s_2((g_2+x_2)/n_2)^\star} \phi(g(x)), \tag{4.18}$$

where $s_1, s_2 \in \{0, 1\}$ determine the chosen action and $(\,\cdot\,)^\star$ denotes the integral part. The introduced signs do not change (4.15) and modify thus only the internal structure (allowing for the counterparts of the four inequivalent spin structures over $\mathbb{T}^2$), not changing the space geometry itself.

Also, denoting the vectors of the representation space by $L^2(\mathbb{T}_{(n_1,n_2)})$ as square-integrable functions is rather formal, as any function on a finite number of points equipped with the uniform discrete measure is square-integrable. Actually, it serves as a reminder of what is necessary in the undiscretized case, as a tool of comparison.

Continuous tori $\mathbb{T}^2_\theta$

The noncommutative torus is the algebra generated by two unitaries U_1, U_2 subject to the relation

$$U_1 U_2 = \lambda U_2 U_1, \qquad \lambda = e^{i2\pi\theta}, \qquad \theta \in \mathbb{R}. \tag{4.19}$$

More precisely algebra elements a are power series $a = \sum_{kl} a_{kl} U_1^k U_2^l$ with coefficients a_{kl} which vanish faster than any polynomial for $k, l \longrightarrow \infty$. The commutative torus corresponds then to the choice $\theta = 0$.

The representation of the algebra on $\mathcal{H} = L^2(\mathbb{T}^2_\theta)$, with basis $|n_1, n_2\rangle$, $n_k \in \mathbb{Z}$, is given by

$$\begin{aligned} U_1|n_1, n_2\rangle &= \lambda^{n_2}|n_1 + 1, n_2\rangle, \\ U_2|n_1, n_2\rangle &= |n_1, n_2 + 1\rangle. \end{aligned} \tag{4.20}$$

This representation possesses a cyclic separating vector $|0, 0\rangle$.

All of these tori, whether finite projective modules over the commutative torus (for θ rational) or with trivial center (for θ irrational) are continuous in the sense of allowing a continuous $U(1) \times U(1)$-symmetry.

4.4.2 Invariant vacua

A complex structure on $\mathcal{H}$ is a linear map $J : \mathcal{H} \longrightarrow \mathcal{H}$ satisfying:

$$J^2 = -1. \tag{4.21}$$

The complex structure's eigenspaces $\mathcal{H}_+$,$\mathcal{H}_-$ are the spaces of positive and negative frequencies. The corresponding eigenvalue projections are P_+, P_- and the following relationships hold:

$$P_\pm = \frac{1 \mp iJ}{2}. \tag{4.22}$$

A sensible restriction of the freedom in J is to require the fulfillment of the following conditions:

1. **Invariance of the vacuum.** J is invariant under the action of the group G.

2. **Charge conjugation.** There is an invariant anti-linear isomorphism between the eigenspaces of J.

3. **Zeroth order condition.** J is a zeroth order pseudo-differential operator. It means that there is a finite limit to the symbol of the operator J in any direction in Fourier space at infinity.

Given the action (4.17) of the group G on the Hilbert space $\mathcal{H}$, J will be invariant under the action of G if

$$\langle \psi_1 \mid g^{-1}(J)\psi_2\rangle - \langle \psi_1 \mid J\psi_2\rangle = \langle g(\psi_1) \mid Jg(\psi_2)\rangle - \langle \psi_1 \mid J\psi_2\rangle = 0 \tag{4.23}$$

for all $g \in G$ and $\psi_1, \psi_2 \in \mathcal{H}$. For this to hold it suffices to require that J is invariant under the action of its generators V_1, V_2 of G.

The above statements involving Fourier space assume the discrete (inverse) Fourier transform on the discretized circle, of which the torus is an easy 2-dimensional generalization. On $\mathbb{T}_{(n_1,n_2)}$, it is given by

$$\begin{aligned} f_{xy} &= \frac{1}{\sqrt{n_1 n_2}} \sum_{p=0}^{n_1-1} \sum_{q=0}^{n_2-1} \tilde{f}_{pq} e^{(2\pi i/n_1)px} e^{(2\pi i/n_2)qy}, \\ \tilde{f}_{pq} &= \frac{1}{\sqrt{n_1 n_2}} \sum_{x=0}^{n_1-1} \sum_{y=0}^{n_2-1} f_{xy} e^{-(2\pi i/n_1)px} e^{-(2\pi i/n_2)qy}, \end{aligned} \tag{4.24}$$

and may be compared with the (inverse) Fourier transform on the continuous torus:

$$\begin{aligned} f(\phi_1, \phi_2) &= \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \tilde{f}_{mn} e^{im\phi_1} e^{in\phi_2}, \\ \tilde{f}_{mn} &= \frac{1}{2\pi} \int_0^{2\pi}\int_0^{2\pi} f(\phi_1, \phi_2) e^{-im\phi_1} e^{-in\phi_2} d\phi_1 d\phi_2. \end{aligned} \tag{4.25}$$

While for the ordinary circle, the high frequency behavior is given by the limit $n \to \infty$ of the Fourier index, for the discretized circles of the torus $\mathbb{T}_{(n_1,n_2)}$, the high frequency behavior is given by the Fourier indices closest to $(n_i + 1)/2$. For n_i even, there are two such indices, $n_i/2$ and $n_i/2 + 1$ and on those we will assume J to agree.

Discretized torus $\mathbb{T}_{(n_1,n_2)}$

Condition (4.23) can be separated using its discrete Fourier transformed equivalent, since in the Fourier picture, (4.17) becomes:

$$\begin{aligned} \widetilde{g(\phi)}(p) &= \frac{1}{\sqrt{n}} \sum_{x=0}^{n-1} (g\psi)(x) e^{-(2\pi i/n)px} \\ &= \frac{1}{\sqrt{n}} \sum_{x=0}^{n-1} (\psi)(x+g \mod n) e^{-(2\pi i/n)px} \\ &= \frac{1}{\sqrt{n}} \sum_{x=0}^{n-1} (\psi)(x) e^{-(2\pi i/n)p(x-g)} \\ &= e^{(2\pi i/n)pg} \tilde{\phi}(p). \end{aligned} \tag{4.26}$$

We have then from (4.23):

$$e^{(2\pi i/n)(p-q)g} J^q{}_p - J^q{}_p = 0 \qquad \text{for any } p, q, g \in \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2}. \tag{4.27}$$

This is possible only if

$$J^q{}_p = 0 \qquad \text{for all } p \neq q. \tag{4.28}$$

Thus, J is determined by a free choice of complex structures $J^p{}_p$ on complex 2-dimensional subspaces $e^{(2\pi i/n)px} \otimes \mathbb{C}^2$ of $\mathcal{H}$.

To completely characterize the freedom of choice, the compatible complex structures on $\mathbb{C}^2$ can be easily computed by generally solving condition (4.21). The solutions can be given as

$$\pm i \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{4.29}$$

and

$$J = -in^k \sigma_k \tag{4.30}$$

with n^k a unit vector in 3-dimensional Euclidean space and σ_k the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4.31}$$

Clearly, (4.29) does not allow for a charge conjugation as the dimensions of the eigenspaces for the eigenvalues $\pm i$ are different and thus solution (4.29) has to be discarded.

Continuous tori $\mathbb{T}^2_\theta$

Repeating the separation procedure (4.26) for a torus $\mathbb{T}^2_\theta$, we get

$$e^{i\phi(n_1-n_2)m} J^{n_1}{}_{n_2} - J^{n_1}{}_{n_2} = 0 \qquad \text{for any } n_1, n_2, m \in \mathbb{Z} \times \mathbb{Z} \tag{4.32}$$

and J on $\mathbb{T}^2_\theta$ is determined by a free choice of complex structures $J^p{}_p$ on complex 2-dimensional subspaces $e^{i\phi m} \otimes \mathbb{C}^2$, $m \in \mathbb{Z}$ of $\mathcal{H}$, as before.

4.4.3 The soldering form

We get the soldering form directly from the high-energy limit of the positive energy projection in direction

$$n^i = \frac{k^i}{|\vec{k}|}$$

of momentum space, cf. Appendix A.2,

$$\lim_{|\vec{k}|\to\infty} P_+ = \tfrac{1}{2}\,(1 - \vec{\not{n}}\gamma^0). \tag{4.33}$$

The corresponding vacuum complex structure $J = iP_+ - iP_-$ has as its limit then

$$\lim_{|\vec{k}|\to\infty} J = -i\vec{\not{n}}\gamma^0. \tag{4.34}$$

Its existence (in any direction) is assured by the zeroth order condition. In the discretized case, this seems to be an empty condition. That this component is finite is of course automatically assured by the discretization. This idea is however of conceptual value in giving geometric significance to the highest frequency component of J in Fourier space.

Continuous tori $\mathbb{T}^2_\theta$

The Fourier space of the torus $\mathbb{T}^2_\theta$ is $\mathbb{Z}\times\mathbb{Z}$. While this lattice does not have a continuous rotational symmetry, we show that there still is an asymptotic $U(1)$-symmetry.

Consider the space of 1-dimensional rays $(kn_1, kn_2)_{k\in\mathbb{N}}$ in $\mathbb{Z}^2$. These uniquely determine 1-dimensional rays $(rn_1, rn_2)_{r\in\mathbb{R}}$ in $\mathbb{R}^2$. But 1-dimensional rays in the Euclidean geometry of $\mathbb{R}^2$ are parametrized by the unit vectors forming the unit circle S^1 with the symmetry group $U(1)$ and rays coming from rays in $\mathbb{Z}^2$ are dense in this circle.

This set-up allows for an asymptotic symmetry requirement of symmetry of Fourier coefficients by assigning to each ray from $\mathbb{Z}^2$ the limit of Fourier coefficients along that ray at infinity and requiring these limits to define by completion a continuous, $U(1)$-covariant function on S^1 which can be used to define a soldering form through (4.34).

Discretized torus $\mathbb{T}_{(n_1,n_2)}$

In the discrete case, infinity in Fourier space is given by integer points on the boundary of the rectangle

$$I = \left[-\left(\frac{n_1+1}{2}\right)^\star, +\left(\frac{n_1+1}{2}\right)^\star\right] \times \left[-\left(\frac{n_2+1}{2}\right)^\star, +\left(\frac{n_2+1}{2}\right)^\star\right],$$

cf. the following Figure.

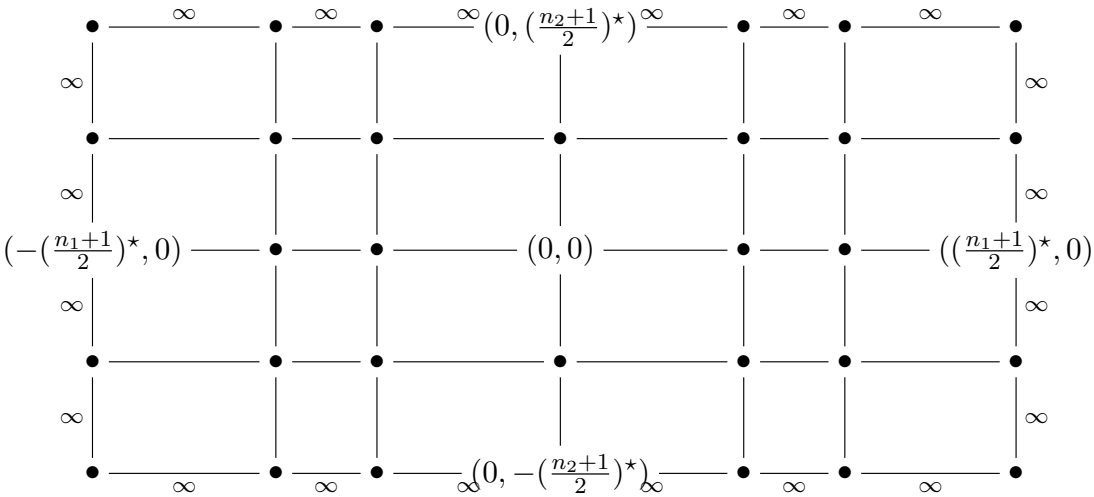


Figure 4.1: **Infinity in finite Fourier space of $\mathbb{T}_{(5,4)}$.** The points on the boundary of the rectangle denoted by ∞ are what is to be considered infinity. Note, that with the particular values $n_1 = 5$, $n_2 = 4$, the infinite points of the upper side of the rectangle are identical with the ones on the lower while the points of the right and left boundary of the rectangle consist of distinct points. The points $(((n_1+1)/2)^\star, 0)$ and $(0, ((n_2+1)/2)^\star)$ are the infinities associated with the two discrete coordinate axes and are used as the high energy limit points for the corresponding coordinate directions.

A clear geometric meaning can be given to the high frequency component of the positive energy projection in the directions of x_1 and x_2, i.e., $P(((n_1+1)/2)^\star, 0)$ and $P(0, ((n_2+1)/2)^\star)$ or directly through the corresponding high energy limit of the complex structure $J(((n_1+1)/2)^\star, 0)$ and $J(0, ((n_2+1)/2)^\star)$, see (A.21).

The choices of these complex structures are free data within our framework and lead to in general noncommuting analogues of Clifford generators, which are according to (4.30):

$$iJ\left(\left(\frac{n_1+1}{2}\right)^\star, 0\right) = n_1^k\sigma_k \qquad iJ\left(0, \left(\frac{n_2+1}{2}\right)^\star\right) = n_2^k\sigma_k. \tag{4.35}$$

Unless $n_1 = \pm n_2$, these operators span the vector space of Clifford generators and the usual spin structure is thus obtained, though with the following restriction.

It is tempting to extend these to some kind of algebra-valued form, as suggested by (A.20), but this idea cannot be applied without further modifications.

First, the linearity with respect to $\vec{n}$ in (A.20) is due to the Dirac operator being a first order differential operator while in a more general physical setting, a pseudodifferential operator is to be expected.

Second, we do not have at our disposal a rotational symmetry in a point of our space as the discretization of the torus destroyed that. This absence of structure is also a problem when dealing with noncommutative spaces, may however possibly be improved upon at least in this case using techniques similar to [42].

Thus the soldering form is not a form in the usual sense of spin manifolds. It does, however, provide a connection between spatial geometry (elementary lattice shifts) and internal degrees of freedom.

* * *

The above example is to be understood as a proof-of-concept: A complex structure given by the positive frequency projection motivated by quantum physics provides a link between spatial geometry and internal degrees of freedom and plays thus in this aspect the role of a soldering form. This was already implicit in the remarkable work of M. H. L. Pryce [35] but not appreciated as a source of geometric information.

The discretization of the example did not change this robust fact while it destroyed the microlocal symmetry of the space in question. The resulting analogues of Clifford generators for elementary lattice shifts are not to be understood in a simple-minded way as components of a form.

Whether a more sophisticated point of view might treat that is an interesting problem for future investigations. The recourse to Fourier theory is at the moment a limitation. Still there are a number of spectral geometries allowing such an approach, notably the noncommutative torus which may be used to test the present ideas in a noncommutative setting.

Compared with Connes's axioms [7], this treatment chose not to start out with the Dirac operator and a fixation of the spin structure and can be seen as a possibility to obtain partial geometric information from concepts of quantum field theory.

Finally, let us remark that our work can also be accounted as an attempt to understand the geometry of negative energy solutions of the free Dirac equation. Another attempt on this problem was recently proposed by E. Trübenbacher, who utilizes just the operator 'sign of the energy', see [41].

Appendix A

Solutions of the Dirac equation on a static spacetime with flat (possibly toroidal) spatial sections

In the following, low space (resp. spacetime) dimensions are considered. While only 2-dimensional space is relevant to our calculations, comparison with other dimensions explains the status of the involved structure since some striking facts on spinors are just coincidences given by a special choice of dimension while other ones have general significance.

A.1 The spin structure and its adjustment to physical requirements

The anticommutation relations for the Clifford algebra are assumed in the form

$$\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2g_{\mu\nu}, \tag{A.1}$$

where $g_{\mu\nu}$ is the metric on the tangent space and the signature is assumed as

$$\operatorname{sign} g_{\mu\nu} = (-\underbrace{+ + \cdots +}_{n}). \tag{A.2}$$

This allows to set up a Clifford bundle acting on a spin bundle with sections ψ. The Dirac equation [39] for such a section ψ is written in the form

$$(\gamma^\mu\partial_\mu - m)\psi = 0. \tag{A.3}$$

Since a number of conventions is available in the literature, it has to be checked that the above settings fit together according to the physical requirements they should satisfy. The signs in the above equation are chosen so that causal propagation is satisfied. This can be checked on flat spacetime, where each solution can be decomposed into plane waves, by showing that the wave vector k_μ of the plane wave $\psi(x) = \psi_0 e^{ik_\mu x^\mu}$ is within the light cone, i.e., $k_\mu k^\mu \leq 0$. This follows from the following calculation:

$$\begin{aligned}(\gamma^\nu\partial_\nu + m)(\gamma^\mu\partial_\mu - m)\psi &= 0\\ (g^{\nu\mu}\partial_\nu\partial_\mu - m^2)\psi_0 e^{ik_\mu x^\mu} &= 0\\ k_\mu k^\mu &= -m^2 \leq 0\end{aligned}$$

There are two natural hermitean inner products on spinors given by the intertwinners of up to isomorphism unique irreducible representations of the Clifford algebra [3]:

$$\gamma_\mu^+ A = A\gamma_\mu \qquad -\gamma_\mu^+ B = B\gamma_\mu \tag{A.4}$$

or more explicitly:

$$\gamma_\mu{}^{\bar{A}}{}_{\bar{B}} A_{\bar{A}B} = A_{\bar{B}A}\gamma_\mu{}^{A}{}_{B} \qquad -\gamma_\mu{}^{\bar{A}}{}_{\bar{B}} B_{\bar{A}B} = B_{\bar{B}A}\gamma_\mu{}^{A}{}_{B} \tag{A.5}$$

The following facts are shown in [3] (our B is their D):

For positive definite g, the A product is positive definite. Since reduction of the spacetime product to the space product changes one type (A, B) into the other (B, A), we have to take B as the correct spacetime spinor product.

For even spacetime dimensions, both A and B exist, in odd spacetime dimensions, just one of them exists. But fortunately in our signature, A always exists for the spatial part while B always exists for the spacetime product. So we can decide for these choices for all $n+1$-dimensional spacetimes. Then the spacetime inner product is B:

$$-\gamma_\mu^+ B = B\gamma_\mu \tag{A.6}$$

and its reduction to space $A = B\gamma^0$ satisfies:

$$\gamma_i^+ B\gamma^0 = B\gamma^0\gamma_i \tag{A.7}$$

We have formal selfadjointness of the operator $\not{D} - m$:

$$B(\phi, (\not{D} - m)\psi) - B((\not{D} - m)\phi, \psi) = \nabla_\mu B(\phi, \gamma^\mu\psi) \tag{A.8}$$

which leads by the application of Stokes' theorem to the invariant inner product on the (phase) space of solutions of the Dirac equation:

$$\langle\phi, \psi\rangle = \int_\Sigma B(\phi, \gamma^\mu\psi)\, d_\mu S = \int_{x^0=0} B(\phi, \gamma^0\psi)\, d^3\vec{x} \tag{A.9}$$

A.2 The Hamiltonian and the positive energy projector

The Dirac equation in flat spacetime (A.3) written as:

$$i\partial_0\psi = \underbrace{(i\gamma^0\gamma^i\partial_i - im\gamma^0)}_{H}\psi, \tag{A.10}$$

allows to read of the Hamiltonian:

$$H = i\gamma^0(\gamma^i\partial_i - m). \tag{A.11}$$

Under Fourier transform:

$$f(x) = \frac{1}{(\sqrt{2\pi})^2}\int \tilde{f}(k)e^{ixk}\, d^n k, \tag{A.12}$$

we have:

$$x^i f(x) \to i\frac{\partial}{\partial k_i}\tilde{f}(k) \qquad \frac{\partial}{\partial x_i} f(x) \to ik_i\tilde{f}(k) \tag{A.13}$$

Denote $E(k) = k^0 = -k_0$, $E(k) = \sqrt{m^2 + \vec{k}^2}$. Then the projectors onto positive and negative frequencies are in the Fourier transform:

$$P_\pm = \frac{1}{2}\left(1 \pm \frac{H}{E}\right) = \frac{1}{2}\left(1 \mp \frac{(\not{\vec{k}} + im)\gamma^0}{\sqrt{m^2 + \vec{k}^2}}\right). \tag{A.14}$$

This projection (expressed in the Fourier picture) is, unlike the ones given in many textbooks, see, e.g., [21], not only onto orthogonal spaces but also an orthogonal projection.

The positive energy projection of a coordinate x^i is $x^i_P = P_+ x^i P_+$.

$$
\begin{aligned}
[x^i_P, x^j_P] &= P_+ x^{[i} P_+ x^{j]} P_+ \\
&= P_+ \underbrace{x^{[i} x^{j]}}_{=0} P_+ - P_+ x^{[i} [x^{j]}, P_+] P_+ \\
&= -x^{[i} \underbrace{P_+ [x^{j]}, P_+] P_+}_{=0} + [x^{[i}, P_+][x^{j]}, P_+] P_+
\end{aligned}
\tag{A.15}
$$

and since

$$
[x^i, P_+] = i \frac{\partial}{\partial k_i} P_+(k) = \frac{i}{2E} \gamma^0 \left(\gamma^i - \frac{\vec{\not{k}} + im}{E^2} k^i \right)
\tag{A.16}
$$

we get

$$
[x^i_P, x^j_P] = -\frac{1}{4E} (\Omega^{ij} - P^i{}_k \Omega^{kj} - \Omega^{ik} P^j{}_k),
\tag{A.17}
$$

where

$$
P^i{}_j = \frac{k^i k_j}{E^2} = \frac{k^i k_j}{m^2 + \vec{k}^2}
\tag{A.18}
$$

$$
\Omega^{ij} = [\gamma^i, \gamma^j]
\tag{A.19}
$$

This projects the spin rotation matrix Ω^{ij} onto the plane orthogonal to $\vec{k}$. This is exactly the case in the high-energy limit (in the massless case), when E is asymptotically equal (exactly equal) to $|\vec{k}|$ and thus $P^i{}_j$ is indeed such a projector. For zero energy, the commutator of the coordinates gives just the spin rotation matrix Ω^{ij}.

In the high-energy limit, one needs at least three dimensions to obtain the spin rotation matrix from the commutators of coordinates. It is easier to get the soldering form directly from the high-energy limit of the positive energy projection in direction

$$
n^i = \frac{k^i}{|\vec{k}|}
$$

of momentum space. Indeed,

$$
\lim_{|\vec{k}| \to \infty} P_+ = \lim_{|\vec{k}| \to \infty} \frac{1}{2} \left(1 - \frac{(\vec{\not{k}} + im)\gamma^0}{\sqrt{m^2 + \vec{k}^2}} \right) = \frac{1}{2} (1 - \vec{\not{n}} \gamma^0)
\tag{A.20}
$$

That this high energy limit exists, i.e., that the symbol of P has a finite limit in momentum space, is basically the requirement that P should be an order zero pseudo-differential operator.

The corresponding vacuum complex structure $J = iP_+ - iP_-$ has as its limit then

$$
\lim_{|\vec{k}| \to \infty} J = -i \vec{\not{n}} \gamma^0,
\tag{A.21}
$$

which justifies interpreting (4.35) as soldering structures.

Conclusion

The thesis dealt with several problems connected with the notion of SQM, a spectral formulation of non-relativistic quantum theory.

In the first, part historical remarks on quantum theory were supplemented with a discussion about some difficulties related to Bohr's formulation of quantum mechanics. Already in 1948, doubting the dogmas of quantum mechanics, R. Feynman tried to reform the framework of quantum mechanics. He attempted to introduce a dynamical system not describable by a Lagrangian or Hamiltonian. In October 1948 he reported to F. Dyson that he failed. Feynman's proof of the Maxwell equations is a no-go theorem. However, after Feynman's death, Dyson published the proof and it was subjected to study from different points of view. We have shown how it was broadly accepted as an interesting research topic and how it led to the notion of SQM.

In Chapter 2, the notion of smoothness was translated into the language of spectral geometry. Then, transporters and their rising operators were introduced and two important physically motivated examples were presented, the (noncommutative) torus $\mathbb{T}^2_\theta$ and a space that is seemingly commutative 1-dimensional at low values of the spectrum of D (with an energy cut-off, a fuzzy circle) and commutative 2-dimensional at high energies, with the two different commutative regimes bridged by a noncommutativity at intermediate energies.

In Chapter 3, we have shown that SQM provides a concise coordinate-free description of nontrivial dynamical systems, which demands only quite general assumptions. In the last section, we have pointed that SQM provides tools for handling a nontrivial topological structure on the configuration manifold, which can affect the spectrum of H.

We have stressed that no axiom in the definition of SQM can at present be weakened without breaking some essential property of the quantum world, except possibly through nontrivial consequences of the positivity axiom for the smoothness condition. If this is the case is to be determined in future research. For any of the considered dynamical systems, the scalarity axiom ensures that Newton's law holds, the smoothness axiom restricts the order of the Hamiltonian from above and specifies the form of canonical commutation relations. The nontriviality and positivity axioms restrict the spectrum of the corresponding Hamiltonian.

In Chapter 4 we have given a detailed historical analysis of early development of Dirac's equations and connected problems. It was noted that the idealized picture of Dirac's heroic achievements should be abandoned and the history of problems with negative energies and its interpretation by the hole theory was put straight. However, our arguments presented in Section 4.4 show, that the solution of the problem of negative energies in Dirac equations by a restriction to positive energies gives for free the soldering form of spin geometry.

Let us finish with an outlook.

A separation of extrinsic and intrinsic structures by means of rising operators u of transporters p would give us the possibility to describe soldering form in a manner applicable to more general situations. E.g., disconcerting ambiguities in an aforementioned, physically motivated model of discrete torus can be naturally removed. This is one of our current goals.

Next we would like to investigate if there could be a connection established between a choice of the projection P_+ on $\mathcal{H} = L^2(\mathcal{Q}, E)$ and a choice of a spin structure on the configuration manifold $\mathcal{Q}$.

Last but not least, we touched in the course of this work on some very interesting facts in the history of soldering structures. It forms one possible direction of enhancing our historical understanding of studied theories.

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Publications of the author's results

Papers concerning the thesis

[A1] J. Kotůlek, Scalar quantum mechanics in (counter)examples, in: *Book of abstracts of the 9th Int. Conf. on Squeezed States and Uncertainty Relations*, Besançon (France), May 2–6, 2005, (CNRS & SFMC, Besançon, 2005) 190.

[A2] J. Kotůlek, Feynmanův důkaz Maxwellových rovnic, in: M. Bečvářová (ed.), *Sborník 28. mezinárodní konference Historie matematiky*, Jevíčko 24.–28. 8. 2007 (Matfyzpress, Praha, 2007), 61–63.

[A3] J. Kotůlek, Nontrivial systems and the necessity of the scalar quantum mechanics axioms, *J. Math. Phys.* **50** (2009), 062101, 1–14. DOI:10.1063/1.3133887

[A4] T. Kopf, J. Kotůlek, and A. Lampartová, Positive energy projectors and spinors, *Electron. J. Theor. Phys.* **7** (2010)(24), to appear.

[A5] J. Kotůlek, Exploring the Scalar Quantum Mechanics: nontrivial systems, topological aspects and the necessity of the axioms, in: *Annual Proceedings of Science and Technology at VŠB-TU Ostrava*, Vol. IV (2010), to appear.

[A6] J. Kotůlek, Problémy Diracovy rovnice 1928–1933, in: *Sborník 31. mezinárodní konference Historie matematiky*, Velké Meziříčí 18.–22. 8. 2010 (Matfyzpress, Praha, 2010), to appear.

Conferences

[C1] 6. setkání matematických fyziků, Olomouc, 19.–20. 3. 2004.

[C2] Workshop on Noncommutative Manifolds, Trieste, Italy, October 18–22, 2004,
poster: Scalar quantum mechanics in (counter)examples.

[C3] 9th International Conference on Squeezed States and Uncertainty Relations Besançon, France, May 2–6, 2005,
poster: Scalar quantum mechanics in (counter)examples.

[C4] 7. setkání matematických fyziků, Brno,
talk: Positive energy projectors (in Czech).

[C5] 28. mezinárodní konference Historie matematiky, Jevíčko 24.–28. 8. 2007,
talk: Feynman's proof of the Maxwell equations; A history (in Czech).

[C6] 29. mezinárodní konference Historie matematiky, Velké Meziříčí, 22.–26. 8. 2008.

[C7] 30. mezinárodní konference Historie matematiky, Jevíčko 21.–25. 8. 2009 (talk in Czech).

[C8] 20. Novembertagung on the history of mathematics, Enschede 4.–8. 11. 2009 (talk).

Seminars

[S1] Feynmanův důkaz Maxwellových rovnic: apokryf o kvantové mechanice, seminář z MA, Opava, 5. 11. 2003.

[S2] Skalární kvantová mechanika v (proti)příkladech, seminář DGA, Opava, 1. 12. 2004.

[S3] Variationality in SQM, 2005

[S4] Spinory na sféře, seminář z MA, 29. 3. 2006.

[S5] Spin structures on the noncommutative torus, seminář DGA, 12. 12. 2008.

[S6] Chovají se pozitivní komutátory pozitivně? seminář DGA, 5. 6. 2009.

Bibliography

[1] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions*, Dover, New York, 1992.

[2] A. Boulahoual and M.B. Sedra, Noncommutative geometry framework and the Feynman's proof of Maxwell equations, *J. Math. Phys.* **44**, 5888–5901 (2003).

[3] P. Budinich and A. Trautman, *The spinorial chessboard* (Springer-Verlag, Berlin, 1988).

[4] J.F. Cariñena, L.A. Ibort, G. Marmo and A. Stern, The Feynman problem and the inverse problem for Poisson dynamics *Phys. Rep.* **263**, 153–212 (1995).

[5] J.F. Cariñena and H. Figueroa, Feynman problem in the noncommutative case, *J. Phys. A* **39**(2006), 3763–3769, arXiv:hep-th/0606008v1.

[6] C.H. Chou, Dynamical equations of spinning particles — Feynman proof, *Physics Letters B* 323 (1994)(2) 147–152.

[7] A. Connes, Gravity coupled with matter and the foundation of non-commutative geometry, *Comm. Math. Phys.* **182**, 155 (1996).

[8] P.A.M. Dirac, The Quantum Theory of the Electron, Part I, *Proceedings of the Royal Society of London, Series A* **117** (Feb. 1, 1928) (No. 778), 610–624; Part II. *Ibidem* **118** (Mar. 1, 1928) (No. 779), 351–361.

[9] P.A.M. Dirac, A theory of electrons and protons, *Proceedings of the Royal Society of London, Series A* **126** (Jan. 1, 1930) (No. 801), 360–365.

[10] P.A.M. Dirac, *The Principles of Quantum Mechanics* (Clarendon Press, Oxford, 1930, 1935_2, 1947_3, 1958_4).

[11] P.A.M. Dirac, Quantised singularities in the electromagnetic field, *Proceedings of the Royal Society of London, Series A* **133** (Sept. 1, 1931) (No. 821), 60–72.

[12] F.J. Dyson, Feynman at Cornell, Phys. Today 42 (1989) 32–38.

[13] F.J. Dyson, Feynman's proof of the Maxwell equations, *Am. J. Phys.* **58** (1990), 209–211.

[14] G. Farmelo, *The Strangest Man: The Hidden Life of Paul Dirac, Quantum Genius* (faber and faber, London, 2009).

[15] V. Georgescu, C. Gérard and J.S. Møller, *J. Funct. Anal.* **216**, 303–361 (2004).

[16] R. Haag and D. Kastler, An Algebraic Approach to Quantum Field Theory, *J. Math. Phys.* **5**, 848–861 (1964).

[17] L. Hardy, Quantum Theory From Five Reasonable Axioms, preprint, arXiv:quant-ph/0101012v4.

[18] S. Helgason, *Groups and Geometric Analysis*, Mathematical Surveys and Monographs **83**, AMS, Providence, 2002.

[19] A. Hermann, K. von Meyenn and V. F. Weisskopf, *Wolfgang Pauli Wissenschaftlicher Briefwechsel*, Band I: 1920–1929 (Springer, New York, 1979); Band II: 1930–1939 (Springer, Berlin, 1985).

[20] A. Holfter, Noncommutative Geometry and Quantization of Spacetimes and Configuration Spaces, PhD. Thesis (in German) Mainz: Johannes Gutenberg University, 2003, [online at http://ubm.opus.hbz-nrw.de/volltexte/2003/476/].

[21] C. Itzykson and J. B. Zuber, *Quantum field theory* (McGraw-Hill, New York, 1980).

[22] A. Jensen, É. Mourre, P. Perry, *Ann. Inst. H. Poincaré Phys. Théor.* **41**, 207–225 (1984).

[23] T. Kato, *J. Funct. Anal.* **96**, 117–129 (1991).

[24] T. Kopf and M. Paschke, Spectral relativistic quantum mechanics, Preprint Series in Global Analysis GA 3/2005 (Mathematical Institute, Silesian University in Opava, January 2005).

[25] T. Kopf and M. Paschke, Generally covariant quantum mechanics on noncommutative configuration spaces, *J. Math. Phys.* **48**, 112101 (2007).

[26] H. S. Kragh, The genesis of Dirac's relativistic theory of electrons, *Archive for the History of Exact Sciences* **24** (1981), 31–67.

[27] H. S. Kragh, *Dirac – A Scientific Biography* (CUP, Cambridge, 1990).

[28] C.R. Lee, Feynman–Dyson proof of the gauge field-equations, *Physics Letters A* 148 (1990) 146–148.

[29] J. Milnor, Eigenvalues of the Laplace operator on certain manifolds, *Proc. Nat. Acad. Sci.* **51** (1964) (4), 542.

[30] W. Moreau and D.K. Ross, Complementary electric Aharonov–Bohm effect, *Phys. Rev. A* **49**, 4348–4352 (1994).

[31] H.P. Noyes, Comment on "Feynman's Proof of the Maxwell Equations" by F. J. Dyson, Preprint SLAC-PUB-5588 (1991).

[32] M. Paschke, Time evolutions in quantum mechanics and (Lorentzian) geometry, preprint, arXiv: math-ph/0301040.

[33] M. Paschke, *Conceptual and mathematical aspects of quantum mechanics* (SU Opava, 2009), [online at http://www.math.slu.cz/studmat/HostProf/PaschkeZS0809.pdf].

[34] M. Paschke and A. Sitarz, On Spin Structures and Dirac Operators on the Noncommutative Torus, *Lett. Math. Phys.* **77**, 317 (2006).

[35] M.H.L. Pryce, The mass-centre in the restricted theory of relativity and its connexion with the quantum theory of elementary particles. *Proc. Roy. Soc. London. Ser. A.* **195**, 62 (1948).

[36] M. Reed and B. Simon, *Methods of Modern Mathematical Physics,* vol. I–IV. Academic Press, New York, 1975–80.

[37] M. Takesaki, *Theory of Operator Algebras,* vol. I., Springer, Berlin, 2001.

[38] S. Tanimura, Relativistic Generalization and Extension to the Non-Abelian Gauge Theory of Feynman's Proof of the Maxwell Equations, *Ann. Phys.* **220**, 229–247 (1992), arXiv: hep-th/9306066.

[39] B. Thaller, *The Dirac Equation* (Springer, Berlin, 1992).

[40] B. Thaller, *Advanced Visual Quantum Mechanics*, Springer, New York, 2005.

[41] E. Trübenbacher, *Electron. J. Theor. Phys.* **7**, No. 23, 355 (2010).

[42] F. Valiquette and P. Winternitz, Discretization of partial differential equations preserving their physical symmetries, *J. Phys. A* **38**, 9765 (2005).

[43] O. Vallée and M. Soares, *Airy Functions and Applications to Physics*, Imperial College Press, London, 2004.

[44] H. Weyl, *Gruppentheorie und Quantenmechanik* (Hirzel, Leipzig, 1928_1, 1931_2). English translation: *The Theory of Groups and Quantum Mechanics* (Methuen, London, 1931; Dover, New York, 1950)