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On a Spectral Formulation of Quantum Mechanics

with an Application to Soldering Form of Spin Geometry

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s aplikací na Infeldovy–van der Waerdenovy symboly spinové geometrie

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1. INTRODUCTION

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, the thesis is divided into an introductory motivation part, where the motivations leading to SQM are studied, 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 exposition in Chapter 1 is based on the author's talk [A7] dealing with Bohr formulation of quantum mechanics and paper [A2], which is a shortened version of the author's talk [A13], dealing with Feynman's proof. In Chapter 2, we describe language of spectral geometry which is employed in the formulation of SQM.

In Chapter 3, 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 non-trivial 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 Chapter 3 forms the core of the work. It 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 [A8] and the 9th International Conference on Squeezed States and Uncertainty Relations Besançon [A10]. Abstract of the latter presentation was published in [A1].

In Chapter 4 we first give a historical account of Dirac's relativistic theory of electron. In this part an extended version of the author's paper [A6] is included. Then we turn to the discussion of soldering structures (in a certain context called Infeld–van der Waerden symbols). We show that a complex structure on phase space provides a soldering form for internal degrees of freedom. The exposition will appear in Electronic Journal of Theoretical Physics, [A4]. This is a joint work with T. Kopf and A. Lampartová.

2. MOTIVATIONS

First, we recall the 'orthodox' formulation of quantum mechanics, which have won recognition through the interpretation of Bohr's Copenhagen school. However, it suffers from some technical difficulties which are only rarely mentioned in elementary physics literature. Therefore, we 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 definition of SQM into the context of generalizations of Feynman's proof.

Then, we describe language of spectral geometry which is employed in the formulation of SQM. 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

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on a Hilbert space \mathcal{H} . Although we are going to modify some attributes of the spectral triples, we recall the features which we build upon.

3. SCALAR QUANTUM MECHANICS

We study an attempt to construct quantum theory with minimal assumptions by M. Paschke [32]. He calls it *scalar quantum mechanics* and he uses purely algebraic definitions of geometric concepts to define quantum mechanics (for one non-relativistic particle) over an arbitrary manifold \mathcal{Q} . More recently, the notion of SQM was discussed in [25] and [33].

It is captured by the algebra $\mathcal{A} = C_0^\infty(\mathcal{Q})$ 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 $\pi : E \rightarrow \mathcal{Q}$.

Definition 1. Let $\mathcal{A} = C_0^\infty(\mathcal{Q})$. 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 $f \in C_0^\infty(\mathcal{Q})$ 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 $\overline{(\cdot)}$ is the closure in the weak topology.

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

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

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

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

holds.

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

Paschke shows that his axioms are sufficient to prove the existence of a Hamiltonian with desired properties [32]:

Theorem 2. *Under the assumptions (a)–(e), there exists for all $t \in \mathbb{R}$ a unique Riemannian metric g_t given by*

$$(1) \quad g_t(da_t, db_t) = -i[a_t, \dot{b}_t],$$

a unique covariant derivative $\nabla(A_t, g_t)$ on the complex line bundle $\pi : E \rightarrow \mathcal{Q}$ and a closed one-form $\phi = \varphi_1 d\varphi_2$ such that for all $b_t \in \mathcal{A}_t$ the following holds:

$$(2) \quad \dot{b}_t = -i[b_t, \Delta(A_t, g_t)],$$

$$(3) \quad \ddot{b}_t = -i[\dot{b}_t, \Delta(A_t, g_t)] - i[b_t, \partial\Delta(A_t, g_t)/\partial t] - i\varphi_1[\varphi_2, \dot{b}_t],$$

where

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

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

$$(4) \quad H(t) = \Delta(A_t, g_t) + \varphi_t.$$

To see more clearly the possibilities and limitations of SQM 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 . First, a free particle on the circle is discussed. The dynamics can be defined by a time evolution operator

$$U(t) = e^{-im^2t}.$$

Next we describe a particle on an expanding circle with the dynamics defined by

$$U(t) = e^{-im^2G(t)},$$

where G is an arbitrary increasing function of time. In this system the Hamiltonian turns up to be time-dependent.

We also study the dynamics of a free particle on S^2 . However, SQM on S^2 can be easily rephrased in the language of harmonic analysis on compact Lie groups and their homogeneous spaces.

Next, the necessity of axioms (a)–(e) is elucidated. We justify each axiom as indispensable and present its physical and/or geometric meaning. 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 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} .

THE SCALARITY AXIOM implies Newton's law. We choose 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

$$(5) \quad \mathcal{A}'_t \supsetneq \overline{\mathcal{A}}_t.$$

The dynamics is defined with the help of the time evolution operator

$$U_{(1)}(t) = e^{-im^2t} \otimes e^{-if^j(t)\sigma_j},$$

where f^j are arbitrary functions and the summation convention on index j has been used.

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. In this sense, equation (3) can be considered as Newton's law.

An operator that illustrates the effects of the condition (5) is of the form $b_{(1)} = b_t \otimes \sigma_i$, where σ_i ($i = 1, 2, 3$) denotes Pauli matrices.

THE SMOOTHNESS AXIOM restricts order of the Hamiltonian. It 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 in fact show that it cannot be satisfied, e.g. by any differential operator of order higher than 2.

The smoothness axiom also specifies the form of the canonical commutation relations.

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. However, by a proper choice of time direction one can always achieve positivity. The nontriviality condition guarantees that the Hamiltonian is at least of second order. Its violation means that there exists a local coordinate $q_t \in \mathcal{A}_t$ such that

$$[q_t, \dot{q}_t] = 0 \quad \text{with} \quad \dot{q}_t \neq 0.$$

Therefore, this would describe an unquantized directions on \mathcal{Q} . Finally, violating both positivity and nontriviality allows indefinite metrics. The resulting Hamiltonian possesses a spectrum with neither a lower nor an upper bound.

Topological aspects of SQM on multiply connected configuration spaces are illustrated on a system inspired by one of the most famous experiments showing topological effects in quantum theory, namely the Aharonov–Bohm effect in its electric form, cf. analysis by W. Moreau and D.K. Ross in [30]. Thus, the results have clear physical background and consequences.

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

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

The states of the system with respect to the coordinate basis are of the form

$$(6) \quad \psi_m(\varphi) = C_1 \text{Ai}(\varphi - E_m) + C_2 \text{Bi}(\varphi - E_m),$$

where Ai and Bi are Airy functions, see, e.g., [1, 43].

The Hamiltonian is then of the form $\hat{H} = P^2 + X$, where X is the local potential of a constant one-form.

We can construct the covariant Laplacian $\Delta = -d_\varphi^2$, but we do not succeed in the constructing of H , as a global non-zero one-form $\phi = d\varphi_t$ 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 2 are not completely met. Hence, no Hamiltonian with the required properties exists.

4. SPINOSE PATHWAY TO GLORY: DIRAC'S ELECTRON THEORY 1928–1933

We open the last Chapter by a historical discussion of Dirac's electron theory, which 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. 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.

It is clear from sources that Dirac had to struggle for his relativistic theory 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.

5. SPIN AND SOLDERING STRUCTURES IN RELATIVISTIC QM

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 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 $\mathbb{T}_{(n_1, n_2)}$. The invariant vacua given by invariant complex structures are discussed. They are described by a complex structure on \mathcal{H} , i.e., a linear map $J : \mathcal{H} \rightarrow \mathcal{H}$ satisfying: $J^2 = -1$.

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.

The high-frequency behavior of J is determined and the soldering form as 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,

$$(7) \quad \lim_{|\vec{k}| \rightarrow \infty} P_+ = \frac{1}{2} \left(1 - \vec{\not{k}} \gamma^0 \right).$$

Corresponding facts on continuous tori are mentioned throughout for comparison. The significance of the presented approach is also discussed.

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.

6. PUBLICATIONS 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.

7. PRESENTATIONS

- [A8] Seminar on Mathematical Analysis, Opava, 5. 11. 2003. Talk: “Feynmanův důkaz Maxwellových rovnic: apokryf o kvantové mechanice”.
- [A9] Workshop on Noncommutative Manifolds, Trieste, Italy, October 18–22, 2004. Poster: Scalar quantum mechanics in (counter)examples.
- [A10] Seminar on Differential Geometry and its Applications, Opava, 1. 12. 2004. Talk: “Skalární kvantová mechanika v (proti)příkladech”.
- [A11] 9th International Conference on Squeezed States and Uncertainty Relations Besançon, France, May 2–6, 2005. Poster: Scalar quantum mechanics in (counter)examples.
- [A12] Seminar on Mathematical Analysis, Opava, 29. 3. 2006. Talk: “Spinory na sféře”.
- [A13] 7. setkání matematických fyziků, Brno. Talk: Positive energy projectors (in Czech).
- [A14] 28. mezinárodní konference Historie matematiky, Jevíčko 24.–28. 8. 2007. Talk: Feynman’s proof of the Maxwell equations; A history (in Czech).
- [A15] Seminar on Differential Geometry and its Applications, Opava, 12. 12. 2008. Talk: “Spin structures on the noncommutative torus”.
- [A16] Seminar on Differential Geometry and its Applications, Opava, 5. 6. 2009. Talk: “Chovají se pozitivní komutátory pozitivně?”
- [A17] 30. mezinárodní konference Historie matematiky, Jevíčko 21.–25. 8. 2009 (talk in Czech).
- [A18] 20. Novembertagung on the history of mathematics, Enschede 4.–8. 11. 2009 (talk).

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