Scalar quantum mechanics in (counter)examples

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Abstract

In this paper we discuss the necessity of the axioms of scalar quantum mechanics introduced by Mario Paschke and clearly demonstrate their meaning. We show that reasonable nonrelativistic quantum mechanics is given exactly with the axioms specified. A system describing the electric Aharonov–Bohm effect is presented too. It illustrates the topological obstructions for the existence of Hamiltonian.

1 Introduction

In 1948 R.P. Feynman showed F.J. Dyson how to prove homogeneous Maxwell equations assuming only Newton's law and commutation relations

$$[x_j, x_k] = 0, \qquad \mathrm{m}[x_j, \dot{x}_k] = \mathrm{i}\delta_{jk}.$$

Feynman was not interested in publishing it, so the proof was only published in 1990 (two years after Feynman's death) with Dyson's editorial comment, see [1]. First it was considered to be a historical feature, but it raised some new questions soon and inspired new research directions. The proof was generalized in several ways, recently for some noncommutative configuration spaces [2, 3], but e.g. a satisfactory relativistic generalization remains still open, cf. [4].

The Feynman proof has inspired M. Paschke in the study of the relation between noncommutative geometry and quantum physics. A generalization of the Feynman proof to arbitrary configuration spaces led him to the attempt on an algebraic definition of quantum mechanics (for one nonrelativistic particle) over an arbitrary manifold $\mathcal{Q}$, see [5]. Paschke calls it scalar quantum mechanics and proves the existence of Hamiltonian with desired properties from his axioms, but the necessity of all axioms remained doubtful. In this paper we work out examples that justify each axiom and present its meaning. Thus, we examine the notion of scalar quantum mechanics (SQM in short). In this meaning, this paper is a sequel to [5].

The paper is organized as follows: Section 2 is devoted to recapitulation of the definition and main properties of SQM. In Section 3 we study two dynamical systems on the circle ($\mathcal{Q} = S^1$) and we perform a construction of Hamiltonian for each of them. One Hamiltonian is time-independent and the other one is time-dependent. These examples demonstrate how SQM works. In Section 4 we consider SQM stepwise with one of the axioms violated letting the other axioms hold and show that some essential property of the quantum world fails to hold. Finally, in Section 5 we illustrate topological obstructions for the existence of the Hamiltonian for multiply connected configuration spaces, more precisely we show that for such $\mathcal{Q}$ that $H^1(\mathcal{Q}) \neq 0$ there need not exist a Hamiltonian with a potential in $\mathcal{A} = \mathcal{C}_0^\infty(\mathcal{Q})$.

2 Scalar quantum mechanics

In this section we review the concept of SQM as given by Paschke in [5]. It is captured by the algebra $\mathcal{A} = \mathcal{C}_0^\infty(\mathcal{Q})$, the set 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 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 all operators that commute with all $a_t \in \mathcal{A}_t$, is just the closure of $\mathcal{A}_t$ in the weak topology,

$$\mathcal{A}_t' = \overline{\mathcal{A}_t} \qquad \forall t \in \mathbb{R}.$$

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

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

(d) POSITIVITY AND NONTRIVIALITY: For every operator a_t the inequality

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

holds. If there exists an operator a_t such that $[a_t, \dot{a}_t] = 0,$ then $\dot{a}_t = 0$.

Note that 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. [5, Lemma 3.2]):

$$g_t(\mathrm{d}a_t, \mathrm{d}b_t) = -\mathrm{i}[a_t, \dot{b}_t], \tag{1}$$

where g_t is the inverse Riemannian metric.

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

Let us recall the main result from [5]:

Theorem 2. (**[5]**) *Under the assumptions* (a)–(d) *there exists* $\forall t \in \mathbb{R}$ *a unique Riemannian metric* g_t *given by* (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* $b_t \in \mathcal{A}_t$ *it holds:*

$$\dot{b}_t = \mathrm{i}[b_t, \Delta(A_t, g_t)], \qquad \textit{(Heisenberg equation of motion)} \tag{2}$$

$$\ddot{b}_t = \mathrm{i}[\dot{b}_t, \Delta(A_t, g_t)] + \mathrm{i}[b_t, \partial\Delta(A_t, g_t)/\partial t] - \mathrm{i}\varphi_1[\varphi_2, \dot{b}_t], \qquad \textit{(Newton's law)} \tag{3}$$

where $\Delta(A_t, g_t)$ *is the covariant Laplacian. If* $\phi = \mathrm{d}\varphi_t$ *is exact, then there exists a Hamiltonian, which is of the form:*

$$H(t) = \Delta(A_t, g_t) + \varphi_t. \tag{4}$$

One may wonder that even very general axioms of Definition 1. specify the admissible dynamics so strictly—spatial derivatives are governed by a second-order Hamiltonian and the time derivatives fulfill the Newton law expressed by (3).

Remark 3. Let x denote the independent variable on the Hibert space $\mathcal{H} = L^2(\mathcal{Q}, E)$. We often need to compute the commutator of an operator $a(x) \in \mathcal{A}$, which acts on states $\psi(x) \in \mathcal{H}$ by multiplication, with some differential operator, particularly with $\mathrm{d}_x := \mathrm{d}/\mathrm{d}x$ and $\mathrm{d}_x^2 := \mathrm{d}^2/\mathrm{d}x^2$. The latter operators are defined on a dense subspace $\mathcal{H}_\infty \subset \mathcal{H}$ and for any vector $\psi(x) \in \mathcal{H}_\infty$ the following operator identities hold:

$$[a, \mathrm{d}_x] = -\mathrm{d}_x a, \tag{5a}$$

$$[a, \mathrm{d}_x^2] = -\mathrm{d}_x^2 a - 2(\mathrm{d}_x a)\mathrm{d}_x. \tag{5b}$$

We use them in the sequel frequently. Moreover, generalizing the latter equations with respect to the order of the derivatives, we get the expression

$$[a, \mathrm{d}_x^m] = -\sum_{q=0}^{m-1} \binom{m}{q} (\mathrm{d}_x^{m-q} a)\mathrm{d}_x^q \qquad \forall m \in \mathbb{N}. \tag{5c}$$

3 Examples of SQM over S^1

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, particularly simple one, we demonstrate the construction of a Hamiltonian, where the topology of $\mathcal{Q}$ does not play any role. Despite of this, the example was chosen to be an essential ingredience in the next constructions of counterexamples. The second example illustrates construction of a time-dependent Hamiltonian.

However, the main intention of this paper is to show the destructive examples, we do not attempt to construct the most general system imaginable.

We use the same setup in this section, namely the algebra $\mathcal{A}_t = \mathcal{C}^\infty(S^1)$, 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 $|\psi\rangle = \sum_m a_m |m\rangle$. Note that the only difference between the two systems resides in the dynamics. In each case it is defined by assigning a particular time evolution operator U.

3.1 Time-independent case without potentials

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

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

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

$$\dot{a}_t = U^\dagger(t)[\mathrm{i}m^2|m\rangle\langle m|, a]U(t). \tag{6}$$

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

$$\dot{a} = \mathrm{i}[a, \mathrm{d}_\varphi^2]. \tag{7}$$

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

- Localizability is obvious.
- Scalarity: The commutant $\mathcal{A}'_t = \mathcal{A}_t$, because $\mathcal{A}$ is commutative $\forall t \in \mathbb{R}$. Closure $\overline{\mathcal{A}_t} = \mathcal{A}_t$ as well, because $\mathcal{A}$ is complete in norm $\forall t \in \mathbb{R}$, so the assertion follows.
- Smoothness: The time evolution is obviously smooth and $\forall a, b \in \mathcal{A}$ it holds

$$\begin{aligned}\mathrm{i}[a, \dot{b}] = \mathrm{i}[a, \mathrm{i}[b, \mathrm{d}_\varphi^2]] &\overset{(5b)}{=} -[a, -\mathrm{d}_\varphi^2 b - 2\mathrm{d}_\varphi b\,\mathrm{d}_\varphi] = 2[a, \mathrm{d}_\varphi b\,\mathrm{d}_\varphi] \\ &\overset{(5a)}{=} -2\mathrm{d}_\varphi b\,\mathrm{d}_\varphi a \in \mathcal{A}_t.\end{aligned} \tag{8}$$

- Positivity: Using (8) we easily get

$$-\mathrm{i}[a_t, \dot{a}_t] = 2\mathrm{d}_\varphi a\,\mathrm{d}_\varphi a = 2(\mathrm{d}_\varphi a)^2, \tag{9}$$

  that is nonnegative.

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

$$\dot{a} \overset{(7)}{=} \mathrm{i}[a, \mathrm{d}_\varphi^2] \overset{(5b)}{=} -\mathrm{i}\,\mathrm{d}_\varphi^2 a - 2\mathrm{i}(\mathrm{d}_\varphi a)\mathrm{d}_\varphi = 0,$$

since $\mathrm{d}_\varphi a = 0$ by (9).

We proceed with constructing the metric on $\mathcal{Q}$. It is given by, cf. [5, Lemma 3.2],

$$\mathrm{i}g_t(\mathrm{d}b, \mathrm{d}c) \overset{(1)}{=} [b, \dot{c}] \overset{(8)}{=} 2\mathrm{i}\ \mathrm{d}_\varphi b\, \mathrm{d}_\varphi c, \tag{10}$$

so the metric $g = \frac{1}{2}$ is static. Taking the total derivative of (7) gives $\ddot{a} = -[[a, \mathrm{d}_\varphi^2], \mathrm{d}_\varphi^2]$. It is consistent with (3) only 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) it follows (cf. also [5, Lemma 3.9]) that $f_t = 0$ and

$$H = -\mathrm{d}_\varphi^2. \tag{11}$$

Remark 4. If the existence of the Hamiltonian is ensured, then 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

$$H(t) = \mathrm{i}\,\frac{\mathrm{d}U(t)}{\mathrm{d}t} \cdot U(t)^{-1}. \tag{12}$$

For the time-independent Hamiltonians we can utilize the Stone Theorem expressed in the formula $U(t) = \exp[\mathrm{i}\,Ht]$. (Hamiltonian is the generator of the time evolution U.) It is then obtained by a simple calculation and it reads

$$H = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} U(t). \tag{13}$$

3.2 Time-dependent case: 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 4., especially (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, cf. (2),

$$\dot{a} = \mathrm{i}\,g_{(\mathrm{A})}[a, \mathrm{d}_\varphi^2]. \tag{14}$$

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

$$-\mathrm{i}[a_t, \dot{a}_t] \overset{(8)}{=} 2g_{(\mathrm{A})}\mathrm{d}_\varphi a\, \mathrm{d}_\varphi a = 2g_{(\mathrm{A})}(\mathrm{d}_\varphi a)^2 \tag{15}$$

is nonnegative if $g_{(\mathrm{A})}$ is nonnegative, that is, if $G_{(\mathrm{A})}$ is increasing, which we assume. We note that the function $g_{(\mathrm{A})}$ governs the velocity of expanding of the circle:

Remark 5. The function $g_{(\mathrm{A})}$ is the inverse Riemannian metric on $\mathcal{Q}$ and it holds

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

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

4 Violating 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 there is 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, therefore we do not violate it and do not explicitly show that it is fulfilled. We work mainly on one-dimensional manifolds S^1 and $\mathbb{R}$ here.

We keep the notation from the Section 3.1 (the objects without subscript and with subscript t), because we use that example in the following constructions.

4.1 Violating the scalarity axiom

The axiom is to be broken by choosing a "larger" Hilbert space $\mathcal{H}$, 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

$$\mathcal{A}_t' \supsetneq \overline{\mathcal{A}_t}. \tag{16}$$

We can construct an example of such a system by modifying the example from Section 3.1 as follows. We consider the algebra $\mathcal{A} = \mathcal{C}^\infty(S^1)$ represented on the Hilbert space $\mathcal{H}_{(1)} = \mathcal{H} \otimes \mathbb{C}^2 = L^2(S^1, S^1 \times \mathbb{C}) \otimes \mathbb{C}^2$.

Note, that all operators from the example of Section 3.1 can be expressed in the form $\mathcal{A} \ni a_{(1)} = a_t \otimes \mathbb{1}_{\mathbb{C}^2}$, where a_t is represented on $\mathcal{H}$. An operator $a_{(1)}$ on $\mathcal{H}_{(1)}$ that illustrates the effects the condition (16), i.e. $a_{(1)} \in \mathcal{A}_t' \setminus \overline{\mathcal{A}_t}$, can be constructed with help of an arbitrary Pauli matrix σ_i ($i = 1, 2, 3$). It is of the form $a_{(1)} = a_t \otimes \sigma_i$, where a_t is again represented on $\mathcal{H}$.

The dynamics is defined with help of the time evolution operator $U(t)$ from Section 3.1 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 4. we can compute the Hamiltonian from (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 Hermitean 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.

- Smoothness: The time evolution is obviously smooth and the required inclusion follows from (8):

$$\begin{aligned} \mathrm{i}[a_{(1)}, \dot{b}_{(1)}] &= \mathrm{i}[a_{(1)}, \mathrm{i}[b_{(1)}, H_{(1)}]] \\ &= -[a_{(1)}, [b_t \otimes \mathbb{1}_{\mathbb{C}^2}, H \otimes \mathbb{1}_{\mathbb{C}^2} + \mathbb{1} \otimes H_{\mathbb{C}^2}]] \\ &= \mathrm{i}[a_t, \underbrace{\mathrm{i}[b_t, H]}_{=\dot{b}_t}] \otimes \mathbb{1}_{\mathbb{C}^2} - [a_{(1)}, \underbrace{[b_t \otimes \mathbb{1}_{\mathbb{C}^2}, \mathbb{1} \otimes H_{\mathbb{C}^2}]}_{=0}] \\ &\overset{(8)}{=} -2\mathrm{d}_\varphi b\, \mathrm{d}_\varphi a \otimes \mathbb{1}_{\mathbb{C}^2} \in \mathcal{A}. \end{aligned} \tag{17}$$

- Positivity: Using (17) and (8) we easily get

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

- Nontriviality follows by the same reasoning as in the example of Section 3.1, since $0_{(1)} = 0 \otimes \mathbb{1}_{\mathbb{C}^2}$.

We shall show that in this system we cannot express the second time derivative of an arbitrary operator $b_{(1)}$ from the first and zeroth one (Newton's law). Let us consider operator $b_{(1)} = b_t \otimes \sigma_i$. From (2) it follows that

$$\dot{b}_{(1)} = -\mathrm{i}[b_{(1)}, H_{(1)}] = \mathrm{i}[b_t, \mathrm{d}_\varphi^2] \otimes \sigma_i + 2\epsilon_{ijk}\dot{f}^j\, b_t \otimes \sigma_k, \tag{18}$$

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

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

Using (18), this indeed becomes

$$\begin{aligned}\ddot{b}_{(1)} =& -[[b_t, \mathrm{d}_\varphi^2], \mathrm{d}_\varphi^2] \otimes \sigma_i + 4\mathrm{i}\, \epsilon_{ijk} \dot{f}^j\, [b_t, \mathrm{d}_\varphi^2] \otimes \sigma_k \\ &+ (4\delta_{in}\delta_{jk} f^j f^n - 4\delta_{ik}(f^j)^2 + 2\epsilon_{ijk}\ddot{f}^j)\, b_t \otimes \sigma_k,\end{aligned} \tag{19}$$

(summation over n, j, k). So there remains an arbitrary function f and its first and second derivatives that stem from $H_{\mathbb{C}^2}$ and we cannot control the time evolution of the system by means of Newton's law (3).

4.2 Violating the smoothness axiom

The smoothness condition is also called the second-order condition, because it guarantees that the Hamiltonian is at the most of second-order. Indeed, a violation of this axiom would admit too wild time evolution of the systems, e.g. such one that is governed by a higher-order Hamiltonian.

In order to show how strange time evolutions are admissible in SQM without the smoothness condition, we construct a system on the bundle $\mathbb{R} \times \mathbb{C} \xrightarrow{\pi} \mathbb{R}$ that is determined by the time evolution operator $U_{(2)}(t) = \exp[it \cdot \exp[-p^2]]$. 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

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

see [7, 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 Theorem, see [7, Theorem IX.6], the Fourier transform map on $\mathcal{S}(\mathbb{R})$ extends uniquely to a linear isometry of $L^2(\pi)$ and consequently $H_{(2)}$ is 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 $a_{(2)} \in \mathcal{A}_{(2)} = \mathcal{C}_0^\infty(\mathbb{R})$,

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

Let us compute the commutators in the coordinate representation, where $p|\psi\rangle = -\mathrm{i}\,\mathrm{d}_x\psi$. Then, we get

$$\begin{aligned}\dot{a}_{(2)}(x) &= -\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}[a_{(2)}(x), \mathrm{d}_x^{2n}] \\ &\overset{(5c)}{=} \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sum_{r=0}^{2n-1}\binom{2n}{r}(\mathrm{d}_x^{2n-r}a_{(2)})\mathrm{d}_x^r.\end{aligned}$$

We proceed with computing the commutator $\mathrm{i}[b_{(2)}, \dot{a}_{(2)}]$:

$$\begin{aligned}\mathrm{i}[b_{(2)}, \dot{a}_{(2)}] &= \mathrm{i}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sum_{r=0}^{2n-1}\binom{2n}{r}[b_{(2)}, (\mathrm{d}_x^{2n-r}a_{(2)})\mathrm{d}_x^r] \\ &\overset{(5c)}{=} -\mathrm{i}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sum_{r=0}^{2n-1}\binom{2n}{r}(\mathrm{d}_x^{2n-r}a_{(2)})\Big(\sum_{s=0}^{r-1}\binom{r}{s}(\mathrm{d}_x^{r-s}b)\mathrm{d}_x^s\Big)\end{aligned} \tag{20}$$

and then show that the latter expression does not fall into $\mathcal{A}$. For this, we should outline that it does not commute with some operator $c_{(2)} \in \mathcal{A}_{(2)}$. But it 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 (20) does not commute even after a finite number of commutators with operators from $\mathcal{A}_{(2)}$!

4.3 Violating the nontriviality axiom

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

$$[a_t, \dot{a}_t] = 0 \quad \text{and} \quad \dot{a}_t \neq 0. \tag{21}$$

We consider SQM over $\mathbb{R}$, i.e. $\mathcal{A}_{(3)} = \mathcal{C}_0^\infty(\mathbb{R}), \mathcal{H}_{(3)} = L^2(\mathbb{R}, \mathbb{R}\times\mathbb{C})$, with the time evolution given by $U_{(3)}(t)|\psi\rangle = \psi(x-t)$. 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 (13) it is generated by the Hamiltonian $H_{(3)} = -\mathrm{i}\,\mathrm{d}_x$. As in the preceding sections, we compute the time derivative $\dot{a}_{(3)}$ of an operator $a_{(3)}$,

$$\dot{a}_{(3)} = -\mathrm{i}[a_{(3)}, -\mathrm{i}\,\mathrm{d}_x] = \mathrm{d}_x a_{(3)}, \tag{22}$$

and test the other SQM-axioms:

- Scalarity: As $\mathcal{A}_{(3)}$ is commutative and closed $\forall t \in \mathbb{R}$, the assertion follows by the same arguments as in Section 3.1
- Smoothness: The time evolution of the system is obviously smooth and $\forall a_{(3)}, b_{(3)} \in \mathcal{A}_{(3)}$ it holds

$$\text{(23)} \qquad \mathrm{i}[a_{(3)}, \dot{b}_{(3)}] = \mathrm{i}[a_{(3)}, \mathrm{d}_x b_{(3)}] = 0 \in \mathcal{A}_{(3)},$$

  because $\mathrm{d}_x b_{(3)} \in \mathcal{A}_{(3)}$ and $\mathcal{A}_{(3)}$ is commutative.
- Positivity: Using (23) we easily get $-\mathrm{i}[a_{(3)}, \dot{a}_{(3)}] = 0 \geq 0$.

We illustrate the behavior of the system on the position operator $x_{(3)}$. From (22) it follows that $\dot{x}_{(3)} = \mathrm{d}_x x_{(3)} = \mathbb{1}$ and the momentum operator is given by $p_{(3)} = \mathrm{m}\mathbb{1}$. Let us compute the canonical commutation relation:

$$\text{(24)} \qquad [x_{(3)}, p_{(3)}] = \mathrm{m}[x_{(3)}, \mathbb{1}] = 0,$$

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 (23) it follows that the metric $g_{(3)}$ is degenerate, even identically zero. Thus, the construction of the covariant Laplacian breaks down, $H_{(3)}$ is not of the form (4) and its spectrum $\sigma(H_{(3)}) = \mathbb{R}$ has neither lower nor upper bound!

4.4 Violating the positivity axiom

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 3.1 Thus, we consider the algebra $\mathcal{A}_{(4)} = \mathcal{C}^\infty(\mathbb{T})$ represented on $\mathcal{H}_{(4)} = L^2(\mathbb{T}, \mathbb{T} \times \mathbb{C})$. The product states are of the form $|\psi\rangle = \sum_{m,n} a_{mn} |m, n\rangle$, where $|m, n\rangle = |\mathrm{e}^{\mathrm{i}m\alpha}, \mathrm{e}^{\mathrm{i}n\beta}\rangle$ and α and β denote the angular coordinates on the corresponding circles.

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

$$U_{(4)}(t)|\psi\rangle = \sum_{m,n\in\mathbb{Z}} a_{mn}(\alpha, \beta) \mathrm{e}^{-\mathrm{i}m^2 t} \, \mathrm{e}^{\mathrm{i}n^2 t} \, |m, n\rangle.$$

As in Section 3.1, we first compute the total time derivative of an arbitrary operator $a_{(4)}(\alpha, \beta)$ that is by virtue of (6) and (7)

$$\text{(25)} \qquad \dot{a}_{(4)} = \mathrm{i}[a_{(4)}, \mathrm{d}_\alpha^2] - \mathrm{i}[a_{(4)}, \mathrm{d}_\beta^2].$$

So we can construct a Hamiltonian with the same procedure as in Section 3.1 or compute it with the help of Remark 4., in particular by eqn. (13). Anyway, it is of the form $H_{(4)} = \mathrm{d}_\beta^2 - \mathrm{d}_\alpha^2$.

Next, we demonstrate that the other axioms are fulfilled. In doing so, let us suppress the index $_{(4)}$.

– Scalarity: The assertion follows by the same argument as in the preceding sections.

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

$$
\begin{aligned}
\mathrm{i}[a, \dot{b}] &= \mathrm{i}[a, \mathrm{i}[b, \mathrm{d}_\alpha^2] - \mathrm{i}[b, \mathrm{d}_\beta^2]] \\
&= -[a, -\mathrm{d}_\alpha^2 b - 2\mathrm{d}_\alpha b\, \mathrm{d}_\alpha] + [a, -\mathrm{d}_\beta^2 b - 2\mathrm{d}_\beta b\, \mathrm{d}_\beta] \\
&= \underbrace{[a, \mathrm{d}_\alpha^2 b]}_{=0} + 2\underbrace{[a, \mathrm{d}_\alpha b\, \mathrm{d}_\alpha]}_{\in\mathcal{A}} - \underbrace{[a, \mathrm{d}_\beta^2 b]}_{=0} - 2\underbrace{[a, \mathrm{d}_\beta b\, \mathrm{d}_\beta]}_{\in\mathcal{A}} \\
&= -2\mathrm{d}_\alpha b\, \mathrm{d}_\alpha a + 2\mathrm{d}_\beta b\, \mathrm{d}_\beta a \in \mathcal{A}.
\end{aligned}
\tag{26}
$$

– Nontriviality follows from the smoothness axiom. From (25) we get

$$
\begin{aligned}
\dot{a} &= \mathrm{i}[a, \mathrm{d}_\alpha^2] - \mathrm{i}[a, \mathrm{d}_\beta^2] \\
&\overset{(5b)}{=} -\mathrm{d}_\alpha^2 a - 2(\mathrm{d}_\alpha a)\mathrm{d}_\alpha + \mathrm{d}_\beta^2 a + 2(\mathrm{d}_\beta a)\mathrm{d}_\beta \\
&= 0,
\end{aligned}
$$

since $\mathrm{d}_\alpha a = 0 = \mathrm{d}_\beta a$ by assumption, cf. Section 3.1

With help of the smoothness axiom (26) we can easily illustrate the violation of the positivity axiom and its consequences. The expression

$$
-\mathrm{i}[a_{(4)}, \dot{a}_{(4)}] = 2(\mathrm{d}_\alpha a_{(4)})^2 - 2(\mathrm{d}_\beta a_{(4)})^2
$$

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

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

and the spectrum of the Hamiltonian $H_{(4)}$ has neither lower nor upper bound!

5 Topological aspects of the SQM on the multiply connected configuration spaces

We have already seen an example of a system on a multiply connected space, namely on S^1, see Section 3.1, 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 perhaps the most famous experiment showing topological effects in quantum theory, namely the Aharonov–Bohm effect in its electric form, see [8]. Thus, the results have clear physical background and consequences.

We again modify the example of Section 3.1 in this construction; we keep the configuration manifold $\mathcal{Q} = S^1$, the algebra of observables $\mathcal{A}_t = \mathcal{C}^\infty(S^1)$ and its representation on the Hilbert space $\mathcal{H} = L^2(S^1, S^1 \times \mathbb{C})$ and change the time evolution only. We set it up namely so as to violate the existence of a Hamiltonian with a potential in $\mathcal{A}$. It reads:

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

The states of the system with respect to the coordinate basis let be of the form

$$\psi_m(\varphi) = \langle\varphi|m\rangle = C_1\,\mathrm{Ai}(\varphi - E_m) + C_2\,\mathrm{Bi}(\varphi - E_m), \tag{27}$$

where Ai and Bi are the Airy functions, see e.g. [6, 9]. Note that the wave functions (21)–(22) in [8] are just asymptotic expansions of Airy functions (27). Here, on $\mathcal{Q} = S^1$, they have to fulfill the following conditions:

$$\psi_m(0) = \psi_m(2\pi), \tag{28a}$$

$$\psi'_m(0) = \psi'_m(2\pi). \tag{28b}$$

Provided these conditions on E hold, the spectrum of H is discrete as in the case without potential, cf. Section 3.1 However, the spectrum cannot be given by a simple closed formula. The Hamiltonian is of the form $H = \widehat{P}^2 + \widehat{X}$. Note, that $\widehat{X} \notin \mathcal{A} = \mathcal{C}^\infty(S^1)$, as it is not continuous in $\varphi = 0$.

In the coordinate representation, where $H = -\mathrm{d}^2_\varphi + \varphi$, 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 Heisenberg equation of motion in the form

$$\dot{a} = -\mathrm{i}[a, H] = \mathrm{i}[a, \mathrm{d}^2_\varphi] - \mathrm{i}[a, x], \tag{29}$$

where the last term is zero by the commutativity of the multiplication of functions in the algebra of functions $\mathcal{F}(S^1) \supset \mathcal{A}$. Next, we compute the metric from (1):

$$g_t(\mathrm{d}b, \mathrm{d}c) \overset{(1)}{=} -\mathrm{i}[b, \dot{c}] \overset{(29)}{=} [b, [c, \mathrm{d}^2_\varphi]] \overset{(8)}{=} 2\mathrm{i}\ \mathrm{d}_\varphi b\, \mathrm{d}_\varphi c, \tag{30}$$

and the metric $g = \frac{1}{2}$ agrees with the metric from Section 3.1!

We can proceed with the construction of H almost up to the end. But in the last step we can not succeed, as the assumptions of the Theorem 2. are not completely met. Indeed, the one-form $\phi = \mathrm{d}\varphi$ is not exact. So, the Hamiltonian with the requied properties does not exist.

Remark 6. There is some correspondence between SQM and Haag–Kastler axioms for quantum field theory in $0+1$-dimensions, see [10]. 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 some similarity in positivity requirement. The main difference is that SQM is not relativistic invariant.

6 Conclusion

We have shown that no axiom in the definition of SQM can be weakened without breaking some essential property of the quantum world. For any dynamical system, the scalarity axiom ensures that Newton law holds, smoothness axiom specifies the form of canonical commutation relations and the nontriviality and positivity axiom restrict the spectrum of the corresponding Hamiltonian. In the last section it has been shown that nontrivial topological structure can affect the spectrum of H as well.

Thus, the SQM is a good candidate for further research, e.g. an analogous definition in the relativistic context could lead to the still missing relativistic Feynman proof.

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