Towards a Usable Ontology for the Quantum World

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Abstract: We present and discuss selected issues related to the problem of representing in a machine-readable way data and knowledge about the quantum level of reality. In particular, we propose a method of creating an ontology for the quantum world. The method uses a mathematical structure of quantum mechanics. We apply the method to obtain a toy ontology corresponding to the Hilbert space formulation of quantum mechanics. We use the terms from the ontology to describe a simple quantum system. We also show how we can use the ontology to create semantic enhancements of scientific publications on quantum mechanics.

1 INTRODUCTION

The term *Ontology* (with uppercase initial) is usually linked to a philosophy where it means a discipline which deals with the nature and structure of reality. Another reading of the term (with lowercase initial) corresponds to computer science, where it means *a formal, explicit specification of a shared conceptualization* (Guarino, 1998). In recent years many ontologies corresponding to various domains have been proposed. They play essential roles in various fields, e.g. knowledge engineering, knowledge representation, database design, information retrieval and extraction. Ontologies (with lowercase initial) can be divided into different kinds according to their level of generality. The most general ontologies are the so-called *top-level ontologies*, describing concepts which are independent of a particular problem or domain, e.g. *space, time, events* and *macroscopic objects*. An exceptional concept among them is *space*. All physical (macroscopic) objects are located in space, which is an ”arena”, a ”support” for them. Consequently, the problem of representing knowledge about space and macroscopic objects has been widely discussed in the literature (Kutz et al., 2003; Borgo et al., 1997; Casati and Varzi, 1996). Recently, an ontology of space, time, and physical entities in classical mechanics has been proposed (Bittner, 2018). The crucial point is that considerations about space and macroscopic objects are based on our *observations*. Indeed, we can observe objects, their positions in space and spatial relations among them. Based on our observations and in general, our sensual perception, we can build an ontology representing given ”part of reality”. According to the ”realism-based” approach, *good* ontologies in the support of the *natural sciences* (and thus also physics) have to be *reality* representations (Smith, 2004). Some authors have expressed doubts about this requirement (Dumontier and Hoehndorf, 2010; Merrill, 2010). For example, Dumontier pointed out that ontologies satisfying this condition face the problem of representing issues which are very important in scientific communication (e.g. hypotheses) and objects which cannot (yet) be shown to exist (e.g. hypothetical elementary particles) (Dumontier and Hoehndorf, 2010). The problem with the ”realism-based” approach is particularly evident when the domain of a considered ontology is not accessible through our sensual perception. This problem happens on the most fundamental level of our world, i.e. on the *quantum level*[1]. We are not able to observe this level directly through our senses. However, despite this, we have successfully explored the quantum world since the theory called *quantum mechanics* (QM) was created. However, the notion of quantum *reality* is still not clear. Surprisingly, it is difficult to say what really (actually) exists on the quantum level. Indeed, in the mathematical structure of QM, nothing is corresponding to the concept of a *quantum object* (Heller, 1994a). In consequence, there are severe problems with the Ontology and interpretations of QM (Bohm and Kaloyerou,

[1]Throughout this paper, we use the terms ’the quantum level’ and ’the quantum world’ interchangeably. The second term frequently appears in the literature to emphasize the difference between the quantum and macroscopic level.

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1987; da Costa and Lombardi, 2014; Busch, 2002; Rudolph, 2006). In this paper, we are going to discuss selected issues related to an ontology (with lowercase initial) of the quantum world. Our motivation is twofold. Firstly, taking into account the multitude of ontologies corresponding to the macroscopic, observable level of reality it seems interesting how to build an ontology for the quantum level. Our second motivation is a more practical one. We are interested in the representation of data (and knowledge) about the quantum world in a way enabling easy integration, sharing and linking the data (Skulimowski, 2014; Skulimowski, 2015). To this end, we need an appropriate ontology for this world. A preliminary and highly incomplete version of a quantum ontology represented in OWL (Web Ontology Langauge) was shortly described in one of our previous papers (Skulimowski, 2010). In this paper, we are going to carry out more detailed research.

The paper is organized as follows. First, to introduce the reader to the amazing quantum world, we present in Section 2 two properties of the quantum world which are contrary to our macroscopic experience. In Section 3, we propose a method for creating a quantum ontology. The method is used in Section 4, where we present a toy quantum ontology and apply it to describe a simple quantum system. We also use terms from the ontology to create RDF links between entities from publication on QM. Finally, concluding remarks are given in Section 5.

2 AMAZING QUANTUM WORLD

The macroscopic world differs significantly from the quantum world. In order to familiarize the reader with the differences, we present below two interesting examples related to *localizability* and *individuality* of entities. These two notions are essential in the ontological analysis and rather evident on the macroscopic level. Let us see how the situation looks on the quantum level.

Localizability. All macroscopic physical objects are *located* in space. The *localization* is an essential property of macroscopic objects. Consequently, (Casati and Varzi, 1996) formulated the following axiom: $\forall x \exists y L(x,y)$ where $L(x,y)$ means that entity x is *exactly located* at region y of space. In his *Formal ontology of space, time, and physical entities in Classical Mechanics* Bittner assumes that from the classical point of view *every particle is located as a unique region of space at every time of its existence* (Bittner, 2018). It turns out that in the quantum world, space is no longer support for any "quantum objects". According to QM, the physical space appears as the set of possible results of a position measurement (which belong to our macroscopic world). That is why Heller proposed that *space should be regarded as the macroscopic entity* (Heller, 1994a). However, from the macroscopic point of view, the behaviour of micro-objects looks very strange. Namely, it turns out that *if at* $t = 0$ *a microscopic particle is strictly localized in a bounded region* y_0 *then unless it remains in* y_0 *for all times, it cannot be strictly localized in a bounded region y, however large, for any* $t > 0$ (Hegerfeldt, 1998). In other words, a particle which is initially strictly localized after that becomes non-localizable because it is *spread over all space*. This result contradicts our macroscopic experience.

Individuality. We can describe macroscopic objects. The description of an object can be seen as a *set of properties* that apply to this object. Based on the properties, we can distinguish objects by comparing their properties. Consequently, using the properties of objects, we can also ascribe *individuality* to them. This statement is evident on the macroscopic level. At the quantum level, the situation is more complicated. Namely, *when two quantum systems, each of which could originally be considered as having a complete set of definite properties, have once interacted, it is generally no longer possible to think of either of them as having a complete set of definite properties of its own* (D'Espagnat, 1999). However, we can assign the set of specific properties to a compound quantum system consisting of these two systems. In quantum world *the best possible knowledge of a whole does not necessarily include the best possible knowledge of all its parts, even though they may be entirely separate and therefore virtually capable of being 'the best possibly known', i.e., of possessing, each of them, a representative of its own* (Schrödinger, 1936). Heller recalls a well-known example: *if two particles interact with each other and then go apart, it is not possible to consider them as two different quantum objects, or even as two parts (subobjects) of the same object each of which would be found in a state independent of the other* (Heller, 1994a) . The two (entirely separated) particles do not have definite properties of its own. We can say that these particles lack the individuality, which is a very characteristic property of macroscopic objects.

The above two examples suggest that our experience obtained in the macroscopic world may not be useful at the quantum level. Consequently, the tools of formal ontology created based on our macroscopic experiences (observations) may be useless in the ontological analysis of the quantum world. So how to create an ontology for the quantum level?

3 QUANTUM ONTOLOGY

The Hidden Structure. We have no direct access to the quantum world. All, we have is the theory called *quantum mechanics* which models the world very precisely, i.e. its predictions agree with the results of numerous experiments. However, despite this agreement, we have severe problems with the understanding of *physical reality* to which the theory refers. This misunderstanding leads to interpretative problems with QM and, in consequence, with the *Ontology* of quantum world (Bohm and Kaloyerou, 1987; da Costa and Lombardi, 2014; Busch, 2002; Rudolph, 2006). Heller (Heller, 1994b) proposed an interesting method for overcoming these problems. The approach uses an observation that *everything we know about the structure of the quantum world we owe to mathematical models of it* (Heller, 1994b). The extraordinary success of QM legitimizes the statement that the *mathematical structure* of QM *strongly interacts* with the *hidden quantum structure*. Consequently, in order to explore the hidden quantum structure, we have to analyze the mathematical structure of QM. The analysis of this structure will give us knowledge about entities and relations it requires to exist. Heller proposes: *let us not bother about the "world" to which quantum mechanics supposedly refers, and let us consider only univers de discours of this theory. By the univers de discours of a physical theory I mean the collection and only the collection of objects, relationships, sets, and so on, which is presupposed by the mathematical structure of this theory* (Heller, 1994a). Thus, we can treat the Heller's approach as the modified Quine's program: we postulate *the existence of only those objects that are presupposed by the mathematical structure of the theory* (Heller, 1994b). It is worth to stress that the reconstruction of the *univers de discours* for the case of empirical theories using complex mathematical structures may not be a simple task. However, this effort can pay off. According to Heller a rigorously reconstructed *univers de discours* of QM can be useful in solving interpretative problems of QM. Moreover, we believe that the *univers de discours* can also be used to obtain an ontology (with lowercase initial) for the quantum world, which can be useful in the creation of semantic enhancements of scientific papers.

Conceptualizations and Ontologies. An ontology corresponds to a *conceptualization*, which is a simplified view of the world we want to represent for some purpose (Guarino, 1998). In order to obtain an explicit specification of a conceptualization, we have to fix a language we want to use to talk about the conceptualization and constrain the interpretations of such a language using suitable *axioms* which usually have the form of a *first-order* logical (FOL) theory (Guarino et al., 2009). A set of such axioms is called an *ontology*. In order to create an ontology for the quantum world, we propose the following 3-steps strategy.

- First, we consider the *univers de discours* $\mathfrak{U}$ of QM as defined by Heller, i.e. the collection of objects, sets, relationships which are presupposed by some mathematical structure of QM, e.g. the Hilbert space formulation of QM.
- Then we choose from $\mathfrak{U}$ essential elements to obtain a *conceptualization*.
- Finally, we create a *set of axioms* for the conceptualization.

One can object that an ontology obtained in this way will be an ontology of QM rather than the ontology of the "real" quantum world. It is true. Notice, however, that in this particular case, the theory is the only way to explore the quantum world. We can say that the theory gives us a unique "access" to the world. Moreover, it is worth to note that the ontology obtained in this way will not be unique. This non-uniqueness is because we can formulate QM by employing several mathematical structures, e.g. Hilbert space formalism, C*-algebraic approach, Feynmann's approach. Each of these structures contains *different collections of objects, relationships, sets and so on* (Heller, 1994a). Therefore, we will obtain different conceptualizations and different ontologies. At first sight, this multitude of quantum ontologies may seem confusing. However, this is not the case taking into account our primary motivation, i.e. usability. Indeed, these various ontologies can be used to enrich with machine-readable data publications using various mathematical formalisms (structures).

Finally, it is worth to mention that if we are interested in the Ontology (with uppercase initial), we have to go one step further. Namely, we have to consider *representation invariants* which are preserved if we change from one mathematical structure to another. According to Heller, the collection of these invariants constitutes the *structuralist ontology* of the quantum world (Heller, 2006).

Axioms for the Quantum World? An ontology is a set of *axioms* in the form of FOL theory for a conceptualization of some domain, which in our case is the quantum world. One can doubt whether it is possible to create such axioms because QM and, in general, physical theories are not *axiomatic systems*. Some terms (names) from logic are indeed used by physicists, e.g. *axioms*, *postulates*, *consequence*, *equivalence* and *contradiction*. However, they cannot be treated in a strictly logical way. Physical theories are rather *models of reality* (Woleński, 1991). Despite this, there have been attempts to formulate strict logical axioms for physical theories (Suppes, 1974; Madarasz et al., 2006). According to the advocates of axiomatization, we can better understand the physical theory by proving a basis of explicit postulates for the theory (Madarasz et al., 2006). Moreover, having axioms for physical theory, one could ask what happens if we change one or more axioms. All axiomatic approaches to QM were sharply criticized by Mielnik, who noticed that axioms in physics *can be very deceptive, even if they look obvious* (Mielnik, 1980). According to Mielnik, strict axiomatic foundations of QM can be an obstacle in the further development of the theory. Putting aside the discussion

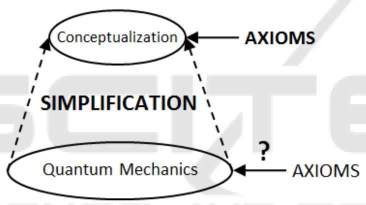

Figure 1: Axioms for ontology, not for quantum mechanics.

about axiomatization of QM let us clarify that we are not going to formulate axioms for QM. Our goal is much more modest. We intend to specify a *conceptualization* for QM and not QM using suitable axioms. We believe that it is possible because a conceptualization is a simplified "model" of the theory (see Fig. 1), i.e. it contains only selected entities and relations from the *univers de discours* of QM.

4 A TOY ONTOLOGY FOR QUANTUM WORLD

In this section, we are going to propose a toy ontology for the Hilbert space formulation of QM. The detailed description of this formulation falls outside the scope of this paper. It can be found in any textbook on QM (see, e.g. (Isham, 1995)). For simplicity, we limit ourselves to the following basic facts:

1. A *state space* of a quantum system is given by a *Hilbert space*.
2. *Observables* (physical quantities) are *self-adjoint operators* defined on the Hilbert space
3. *Vectors* in the Hilbert space represent *states* of a quantum system.
4. Real *eigenvalues* of a self-adjoint operator correspond to *results of a measurement* of observable represented by this operator.
5. The *Schrödinger equation* describes the *time evolution* of quantum states.

Let us now consider the *univers de discours* for this formulation of QM. According to Heller it contains *objects*, *relationships* and *sets* which are required by the mathematical structure (Heller, 1994a). Listing all elements of this collection is not an easy task. Below, we limit ourselves to the following set of relations, which are the backbone of the Hilbert space formulation of QM and are usually present in publications on this formulation:

1-ary relations:

- $StateSpace(x)$ - x is a state space.
- $HilberSpace(x)$ - x is a Hilbert space.
- $VectorHS(x)$ - x is a vector is a Hilbert space.
- $Observable(x)$ - x is an observable.
- $SAOperator(x)$ - x is a self-adjoint operator[2].
- $State(x)$ - x is a state.
- $SchroedingerEq(x)$ - x is a Schrödinger equation.
- $Hamiltonian(x)$ - x is a Hamiltonian operator.
- $Real(x)$ - x is a real number.

Binary relations:

- $isElementOf(x,y)$ - a state x belongs to a state space y.
- $x \perp y$ - a state x is orthogonal to a state y.
- $hasEigenVal(x,y)$ - an operator x has an eigenvalue y.
- $hasEigenV(x,y)$ - an operator x has an eigenvector y.
- $hasMeasurementR(x,y)$ - a result of a measurement of an observable x may be y.
- $correspondsToEigenV(x,y)$ - an eigenvalue x corresponds to eigenvector y
- $solOfSchroedinger(x,y)$ - a state x is the solution of a Schrödinger equation y.

Tenary relations:

- $commutator(c,x,y)$ - c is the result of the commutator of x and y.

[2]For brevity, we consider only self-adjoint operators.

- $meanValue(x,y,z)$ - an observable x in a state y has the expected value z.
- $uncertainty(d,o,x)$ - d is the dispersion of an observable o in a state x.
- $timeEvolution(x,y,h)$ - x is a state which evolved from a state y according to Hamiltonian h.

4-ary relation:

- $probabilityOfR(p,r,y,o)$ - p is the probability of obtaining result r in a state y, in the measurement of o.

In order to specify our conceptualization more precisely, we propose the following simple set of axioms specifying the quantum domain[3].

Taxonomic information[4]:

$StateSpace(x) \rightarrow HilberSpace(x)$
$Observable(x) \rightarrow SAOperator(x)$
$State(x) \rightarrow VectorHS(x)$
$Hamiltonian(x) \rightarrow Observable(x)$
$hasMeasurementR(x,y) \rightarrow hasEigenVal(x,y)$

Domains and ranges:

$x \perp y \rightarrow State(x) \wedge State(y)$
$hasEigenVal(x,y) \rightarrow SAOperator(x) \wedge Real(y)$
$hasEigenV(x,y) \rightarrow SAOperator(x) \wedge VectorHS(y)$
$isElementOf(x,y) \rightarrow State(x) \wedge StateSpace(y)$
$hasMeasurementR(x,y) \rightarrow Observable(x) \wedge Real(y)$
$solOfSchroedinger(x,y) \rightarrow$
$State(x) \wedge SchroedingerEq(y)$

We can specify the properties of the relations:

- Symmetry: $\perp$.
- Irreflexivity: $isElementOf$, $hasMeasurementR$, $hasEigenVal$, $hasEigenV$, $correspondToEigenV$, $solOfSchroedinger$, $\perp$.
- Asymmetry: $isElementOf$, $hasMeasurementR$, $hasEigenVal$, $hasEigenV$, $correspondToEigenV$, $solOfSchroedinger$.

Using the above basic set of relations, we can formulate more axioms, e.g.:

$$hasEigenV(x,y_1) \wedge hasEigenV(x,y_2) \wedge y_1 \neq y_2 \Rightarrow y_1 \perp y_2$$

$$hasMeasurementR(x,y) \Rightarrow hasEigenVal(x,y)$$

$$correspondsToEigenV(x,y) \Rightarrow \exists z \; SAOperator(z) \wedge hasEigenVal(z,x) \wedge hasEigenV(z,y)$$

[3]For brevity, we present only selected axioms.

[4]In the formulas below, we omit the quantifiers $\forall x \forall y$ ...

The proposed conceptualization contains only the most essential entities from the Hilbert space formulation of QM. Note that, it consists of physical entities (e.g. *Observable*) and purely mathematical (e.g. *hasEigenVal*) entities. It is quite reasonable taking into account that the conceptualization we obtained from the mathematical structure of QM. In the future, all mathematical relations and axioms should be taken from the appropriate mathematical ontology. We can also observe that the ontology contains nine classes (1-ary relations), but there are only five taxonomic relations. Moreover, note that for almost all binary relations *domains* differ from *ranges*. The reason for this is that the structure of QM contains relations between entities of different types. Consequently, there is only one *symmetric* relation ($\perp$). All other relations are *irreflexive* and *asymmetric*. It is interesting, that the proposed conceptualization does not contain any *transitive* relation (the *transitivity* is usually required in the case of *mereological* relations). Note also that, apart from *binary* relations there are also *ternary* relations (e.g. *commutatorOf, meanValue*) and even one 4-ary relation (*probabilityOfR*). These relations are fundamental in the formalism of QM.
It is worth to mention that in our ontology, there is no quantum counterpart of the predicate L related to the location in space mentioned in Section 2. The result obtained by Hegerfeldt tells us something about the *expected value* of a particular *self-adjoint operator N* (corresponding the probability to find a particle or system inside some region V) (Hegerfeldt, 1998). Consequently, formalization of the result would require the use of the predicate $meanValue$, the operator N and some quantum state x.

Example. Let us now try to use the terms from our ontology to represent knowledge about some quantum system. To this end we consider the electron described by the *Hamiltonian* operator $\hat{H} = \hat{1} + \alpha\sigma_y$ where $\alpha \in \mathbb{R}$,

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (1)$$

is the Pauli spin-matrix and $\hat{1}$ is the unit 2×2 matrix. Hilbert space for this system is $\mathbb{C}^2$. The *spin operators* for this system are given by:

$$\hat{S}_x = \frac{\hbar}{2}\left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right), \; \hat{S}_y = \frac{\hbar}{2}\left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right), \; \hat{S}_z = \frac{\hbar}{2}\left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right) \quad (2)$$

After some calculations one can show that[5] (Isham, 1995):

[5]The detailed explanation of this quantum system falls outside the scope of this paper. All we want to show is that the knowledge about this quantum system can be represented using terms from the proposed ontology.

- The possible *results of measurement* of the *observable* $\hat{H}$ are $1 \pm \alpha$.
- The Schrödinger equation:

$$i\hbar \frac{d|\psi_t\rangle}{dt} = \hat{H}|\psi_t\rangle \tag{3}$$

- If the *state* at some time $t = 0$ is $|\psi_0\rangle = \binom{1}{0}$ then at some later time t the *state* will be:

$$|\psi_t\rangle = e^{-it/\hbar} \begin{pmatrix} \cos(\alpha t/\hbar) \\ \sin(\alpha t/\hbar \end{pmatrix} \tag{4}$$

(solution of equation (3))

- The *probability of obtaining* result $\hbar/2$ (corresponding to state $|\uparrow\rangle$) in state (4) is given by:

$$Prob(S_z = \frac{\hbar}{2}; |\psi_t\rangle) = |\langle\uparrow|\psi_t\rangle|^2 = cos^2 \frac{\alpha t}{\hbar} \tag{5}$$

Similarly:

$$Prob(S_z = -\frac{\hbar}{2}; |\psi_t\rangle) = |\langle\downarrow|\psi_t\rangle|^2 = sin^2 \frac{\alpha t}{\hbar} \tag{6}$$

- The *expected result* of S_x in the state (4):

$$\langle S_x \rangle = \frac{\hbar}{2} sin \frac{2\alpha t}{\hbar} \tag{7}$$

- The uncertainty in state (4):

$$\triangle S_x = \frac{\hbar}{2} \left| cos \frac{2\alpha t}{\hbar} \right| \tag{8}$$

- The commutator of $\hat{S}_x$ and $\hat{S}_y$

$$[\hat{S}_x, \hat{S}_y] = \frac{\hbar^2}{2} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i\hbar\hat{S}_z \tag{9}$$

We can see that the above description of the quantum system contains formulas of two kinds:

A. *expression* = *numerical value* (depending on a certain parameter)

B. *expression* 1 = *expression* 2

Examples of type A formulas are: (5), (6), (7), (8). Examples of type B formulas are: (1), (2), (3), (4) (9). Below we accept the following convention: for formulas of type A, the use of a formula number `#n` means the reference *to a numerical value* on the right side of the formula. For formulas of type B, the use of a formula number `#n` means the reference *to the whole formula*. For example, by `#6` we refer to the *value* $sin^2 \frac{\alpha t}{\hbar}$, by `#1` we refer to the *formula* $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$.

The following symbols appear in the description of our quantum system:

$$\hat{H}, \mathbb{C}^2, \hat{S}_x, \hat{S}_y, \hat{S}_z, 1+\alpha, 1-\alpha,$$
$$\binom{1}{i}, \binom{1}{-i}, |\psi_0\rangle, |\psi_t\rangle, \frac{\hbar}{2}, -\frac{\hbar}{2}$$

Below we use the following simplified (text) versions of these symbols:

```
#H,#C^2,#S_x,#S_y,#S_z,#1+alpha,#1-alpha,
#(1_i),#(1_-i),#psi_0,#psi_t,
#hbar_div_2,#-hbar_div_2
```

Using the vocabulary from our simple ontology, we can describe the quantum system presented above as follows:

```
Hamiltonian(#H)
Observable(#S_x),Observable(#S_y)
Observable(#S_z)
hasMeasurementR(#H,#1+alpha)
hasMeasurementR(#H,#1-alpha)
correspondsToEigenV(#1+alpha,#(1_i))
correspondsToEigenV(#1-alpha,#(1_-i))
SchroedingerEq(#3)
solOfSchroedinger(#4,#3)
timeEvolution(#psi_t,#psi_0,#H)
meanValue(#S_x,#psi_t,#7)
commutator(#S_z,#S_x,#S_y)
isElementOf(#psi_0,#C^2)
isElementOf(#psi_t,#C^2)
probabilityOfR(#5,#hbar_div_2,#4,#S_z)
probabilityOfR(#6,#-hbar_div_2,#4,#S_z)
uncertainty(#8,#S_x,#psi_t)
```

Exemplar inferences:

```
StateSpace(#C^2),HilbertSpace(#C^2)
Observable(#H),SAOperator(#H)
State(#psi_0),State(#psi_t)
Real(#1+alpha),Real(#1-alpha)
State(#4), SchroedingerEq(#3)
SAOperator(#S_x)
SAOperator(#S_y)
SAOperator(#S_z)
hasEigenVal(#H,#1+alpha)
hasEigenVal(#H,#1-alpha)
```

The ontology proposed in this paper is very simple and require further work. However, the ontology is enough to show that terms from it can be used to create *semantic enhancements* for scientific publications on QM. There is a vast amount of literature on semantic publishing and semantic enhancements of scientific publications (Shotton et al., 2009; Shotton, 2009). In general, the enhancements facilitate the integration of data and knowledge between articles. Below, we show that the terms from the proposed ontology can be used to create RDF (Resource Description Framework)[6] statements. For this purpose, the ontology should be represented in OWL (Web Ontology Language)[7] language. For reasons of space, we do not address the issue in this paper. It was preliminarily discussed in our previous paper (Skulimowski, 2010).

[6]https://www.w3.org/RDF/

[7]https://www.w3.org/OWL/

Moreover, we need a method of assigning URIs (Uniform Resource Identifiers) to entities from scientific papers. For this purpose, we can use the URL of a paper and a *local name* of an entity from the paper: `articleURL#LocalName` (Skulimowski, 2014). Because all the entities considered in the above example come from the same publication, we below omit `articleURL`. For simplicity, we also omit the prefix related to the namespace of the proposed ontology. Below, we present examples of RDF statements using relations from the proposed ontology.

- *Unary relations* allow describing types of entities from scientific papers on quantum mechanics. For example[8]:

```
<#S_x> a :Observable .
<#H> a :Hamiltonian .
<#3> a :SchroedingerEq .
```

- *Binary relations* allow representing relations between entities from scientific publications. For example:

```
<#psi_0> :isElementOf <#C^2> .
<#H> :hasMeasurementR <#1-alpha> .
<#4> :solOfSchroedinger <#3> .
```

- *N-ary relations*, where $N > 2$ - it turns out that many important concepts of quantum mechanics correspond to relations which link more than two entities e.g.: $meanValue(x,y,z)$, $commutator(x,y,z)$. In OWL n-ary relation can be represented as classes with n properties. Instances of such class correspond to instances of the relation (W3C, 2006). For example, the commutator relation we can represent as follows:

```
_:c a :Commutator;
 :element1 <#S_x> ; :element2 <#S_y> ;
 :value <#S_z> .
```

  The mean value relation:

```
_:m a :MeanValue; :ofObservable <#S_x> ;
      :inState <#psi_t> ;
      :value <#7> .
```

  Please note that we need several new relations to implement the above two relations formally.

5 FINAL REMARKS

In this short paper, we have proposed a method for obtaining a semantic ontology for the quantum world. The method uses the fact that the full knowledge we have about the quantum level we owe to quantum mechanics (Heller, 1994a). Consequently, we propose to create an ontology from the *univers de discours* of this theory defined as the collection of objects, relationships, sets and so on which are presupposed by the mathematical structure used in the theory (Heller, 1994a). An ontology obtained by using the proposed method is not unique because quantum mechanics can be formulated using various mathematical structures. Ontologies of QM corresponding to these structures can be used to create semantic enhancements and RDF links between entities from scientific papers using various formalisms. Moreover, it is worth to mention that the ontologies obtained using the proposed method do not face the problem of *hypothetical entities* pointed out by critics of *realism-based* approaches in natural sciences (Dumontier and Hoehndorf, 2010). Such entities, even if only hypothetical, can be usually represented somehow in the mathematical formalism of the theory.

We have applied the proposed approach to the Hilbert space formulation of QM and presented a toy ontology based on this formalism. The reason for choosing this formulation was that most of the articles on QM use it. However, taking into account the goal we want to achieve (create an ontology as a set of axioms in a FOL language), the more natural candidate for creating an ontology is another "formulation" of QM namely called yes-no measurements (Mielnik, 1968). The point is that yes-no measurements possess specific properties analogous to those of logical systems. That is why their set is called *quantum logic*.

Future studies should focus on the development of a more mature ontology for Hilbert space formulation of QM and other formalisms of QM (e.g. C*-algebraic approach, Feynmann's approach). The toy ontology presented in this paper is very simple and contains only selected terms from the Hilbert space formulation of QM. If we want to create more precise semantic enhancements for advanced publications on QM, we have to broaden the set of relations and axioms in the ontology. We believe that to create a useful ontology of quantum mechanics (used, for example, in creating semantic enhancements), the explicit formalization of this theory is not required. Nevertheless, the axiomatization of quantum mechanics remains an interesting research problem.

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[8]Throughout this paper, we use Turtle syntax for RDF (https://www.w3.org/TR/turtle/).

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