An OWL Ontology for Quantum Mechanics

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Abstract. An OWL ontology for quantum mechanics is presented in short. The motivation for its development, structure and characteristic features are depicted. In particular, some essential concepts from the ontology are described. Finally, some problems encountered during the development of the ontology are discussed.

1 Introduction

The main aim of the Semantic Web is to make the information on the World Wide Web more accessible to machines [1]. The key role in the Semantic Web is played by ontologies which are formal conceptualizations of domains [2]. There exists a variety of ontologies connected with many domains (see e.g. [3]). However, it is difficult to find among them ontologies corresponding to physics and in particular an ontology for quantum mechanics. One of the reasons of this fact may be that quantum mechanics is a mathematically and conceptually complicated theory. For this reason, it is not an easy task to create the ontology. Though, such an ontology would be useful taking into consideration the dynamical development of quantum mechanics. A dozen of new articles is published every day (see `http://arXiv.org` preprint archive), and experiments concerning quantum mechanics are performed in many laboratories spread all over the world. The number of publications about quantum mechanics and related disciplines implies some difficulties for scientists in getting and analyzing the available information. The existing search-tools are insufficient because the knowledge gathered in archives such as `http://arXiv.org` is not machine processable and interpretable similarly as the knowledge gathered in today's Web pages. In order to change the situation and to make the knowledge of quantum mechanics available for machines we need an appropriate ontology. The ontology which will provide a framework for automatic processing and integration of data connected with quantum mechanics. What is more, it will enable a knowledge-based searching and an annotation of experimental data with terms from the ontology. And this will facilitate sharing and reuse of the data. It is especially important because of the fact that quantum mechanics has an impact on many other disciplines. This is what the paper is devoted to. The first version of an ontology for quantum mechanics is presented. Moreover, its structure, characteristic features and some problems which occurred in the process of its development are described.

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2 Assumptions

Our aim is to build an OWL (Ontology Web Language)[4] ontology for quantum mechanics which will model the main concepts that appear in the theory and can be useful in the Semantic Web. To achieve this goal, we assume that quantum mechanics can be treated as a set of individuals (objects) and a set of relations (in general n-ary) which join these individuals. Moreover, some individuals may possess attributes. These assumptions are very important. In an OWL ontology individuals with similar characteristics can be grouped in *classes*; relations correspond to OWL *object properties* and attributes to OWL *datatype properties*. At first sight, obtaining such a picture of quantum mechanics is not obvious. This is mainly because the theory is conceptually and mathematically very complicated [5]. However, the picture becomes to appear when we look at quantum mechanics *from some distance*. This means that we are mainly interested in *classes of objects* used in quantum mechanics and in *relations* between them. We initially pass over some mathematical details of the theory, which may cover the picture. For example, we define a class called *LinearOperator* grouping all linear operators on a Hilbert space. However, we omit in the definition mathematical details which precise what it means for an operator *to be linear*. Similarly, we define an object property called *hasAdjoint* which connects a linear operator defined on a Hilbert space with its adjoint. In this case, mathematical details corresponding to the definition of an operator adjoint are also omitted. We limit ourselves to defining an *object property*. The property has a given name and its characteristics are described in so far as it is possible in OWL.

After building such a *preliminary ontology* we may try to take into account, omitted previously, mathematical details of the theory. It turns out, however, that in many cases the details cannot be modeled in OWL (see Section 4). As a consequence an ontology obtained in this way will model quantum mechanics only approximately. Nevertheless, we think that it will be useful in applications.

3 quONTOm

A preliminary version of an OWL ontology for quantum mechanics named *quONTOm* is available on: `http://merlin.phys.uni.lodz.pl/quONTOm/`. The ontology is written using Protégé 4.1 ontology editor.

Actually the ontology is contained in one OWL document. Aside from quantum mechanical concepts, the ontology contains concepts which are not parts of quantum mechanics, i.e. they are, for example, purely mathematical objects and should be contained in an ontology for mathematics. Unfortunately, to our best knowledge, an appropriate ontology for mathematics, which could be imported and used in *quONTOm* does not exist. The situation is similar for physical concepts. In the future the concepts will be separated from the ontology and become parts of auxiliary ontologies.

The ontology is at the moment incomplete and will be gradually developed towards a more complete form. In spite of this we may try to say something about the structure and the characteristic features of the ontology.

3.1 Names

According to the definition, an ontology provides shared vocabulary used to describe entities in some domain of interest [7]. It happens in some domains that it is not easy to establish this *shared vocabulary* mainly due to ambiguities in the meaning of terms. Fortunately, in the case of quantum mechanics physicists are in agreement on the meaning of terms. So there is no problem with names of concepts in the ontology.

3.2 Classes

There are various kinds of objects in quantum mechanics. Some of them are purely mathematical objects (e.g. linear operators), some objects really exist (e.g. particles). The objects can be grouped in classes. It turns out however that it is very often impossible to establish *subsumption relation* between classes. As a consequence the *class hierarchy* of the ontology will be rather flat. However, the ontology will be rich in other relations.

3.3 Properties

In OWL, a property is a binary relation. Instances of properties link two individuals. However, in quantum mechanics we meet not only binary relations but also n-ary relations. It turns out that many important concepts of quantum mechanics correspond to n-ary relations where $n > 2$. Consider, for example, the following statement which can be found in any book on quantum mechanics: commutator of operators O_1 and O_2 is equal to 0. This statement falls under the category of 3-ary relations. In general an n-ary relation can be represented in OWL as a class with n properties [6]. Instances of a such class correspond

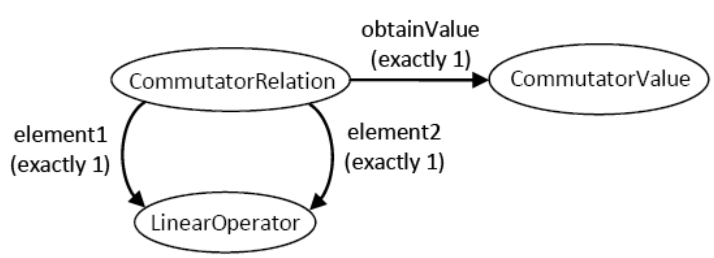

Fig. 1. 3-ary relation corresponding to a commutator.

to instances of the relation. Class properties provide links to each argument of the relation. In *quONTOm* an 3-ary relation is used, for example, to represent a commutator (Fig. 1):

```
Class: CommutatorRelation
SubClassOf:
    element1 exactly 1 LinearOperator
    element2 exactly 1 LinearOperator
    obtainValue exactly 1 CommutatorValue
```

In the case of *quantum evolution* a 5-ary relation is needed. The evolution of a state ψ (*initalState*) is generated by (*generatedBy*) a Hamiltonian H, starts at t_1 (*startTime*) and ends at t_1 (*endTime*). The result of the evolution is a state ϕ (*finalState*). Manchester syntax:

```
Class: TimeEvolution
SubClassOf:
    finalState exactly 1 State
    initialState exactly 1 State
    isGeneratedBy exactly 1 Hamiltonian
    endTime exactly 1 xsd:float
    startTime exactly 1 xsd:float
```

Other fundamental concepts are also represented by n-ary relations (where $n > 2$), for example *quantum measurement*. It seems that as the ontology will be developed the number of such relations will increase.

3.4 Characteristics of Properties

Relations between concepts in quantum mechanics determine characteristics of corresponding properties in the ontology. We observe that there is a numerous set of *functional* properties in the ontology e.g. *hasAdjoint* - a property relating an operator to its adjoint, *isRepresentedByOperator* - a property relating an observable to the corresponding self-adjoint operator, *startTime* - a property relating some initial time to the evolution. There are also numerous classes of objects that have exactly 1 value for some property (e.g. *SelfAdjointOperator, Measurement*). By contrast *transitive* and *symmetric* properties are rather rare. This is mainly because, in quantum mechanics binary relations between objects of the same kind are rare (e.g. a commutation relation between two operators). It seems that the development of the ontology will not significantly change this situation. We also note that the ontology does not contain a merological relation *a partOf*. This is due to the specific domain of the ontology. In the case of objects existing (and extended) in space a *partOf* relation seems to be very natural. For the case of mathematical objects which are not placed in space it is difficult to talk about such a relation. Admittedly, in the ontology a relation *isElementOf* is defined. However, the relation is *asymmetric* and *irreflexive* but not *transitive*: a state *isElementOf* a Hilbert space, the Hilbert space *isElementOf* a family of Hilbert spaces but it is not true that the state *isElementOf* the family of Hilbert spaces. Finally, it is worth to notice that the majority of relations in the ontology are those which are *asymmetric* and *irreflexive*.

3.5 Benefits of OWL 2

During the development of the ontology it turned out that some relationships between concepts in quantum mechanics cannot be represented in OWL 1. To represent them we have to use OWL 2. For example, we can define properties as a composition of other properties. Thanks to this we are able to define a result of a measurement as an eigenvalue of a self-adjoint operator representing some observable.

```
ObjectProperty: measurementResult
SubPropertyChain:
    measurementOf o isRepresentedBy o hasEigenValue
```

In a similar way, we define an object property corresponding to a quantum mechanical state reduction. And these are not the only benefits of using OWL 2.

It happens very often in mathematics that a property of objects belonging to some set is used to define some subset of objects. For example, in a set of matrices we may consider a property *transpose* which assign the transpose matrix to a matrix. Using the property we can define a symmetric matrix as a matrix that is equal to its *transpose*. For linear operators on a Hilbert space we consider a property *adjoint* assigning the adjoint to an operator. *An operator is self-adjoint if it is equal to its own adjoint.* In order to manage such a definition in *quONTOm* we use a *self restriction* offered by OWL 2. First, we introduce a *hasAdjoint* object property and then we define a class of self-adjoint operators (*SelfAdjointOperator*) as linear operators that are related to themselves via the *hasAdjoint* property. Manchester syntax:

```
Class: SelfAdjointOperator
EquivalentTo: hasAdjoint some Self
```

In quantum mechanics there are also objects which can be uniquely identified by some set of attributes. For example, a *complex number* is uniquely identified by its *real* and *imaginary* parts. In such cases we can use *keys* available in OWL 2.

OWL 2 supports restrictions of datatypes by facets, as in XML Schema. Thanks to this we can define new datatypes. In *quONTOm* we define a datatype *probValue* by constraining the datatype *float* to values between (inclusively) 0 and 1. The datatype is very important in *quONTOm* taking into account that quantum mechanics is probabilistic in nature.

4 Some Problems

In this paper we have briefly described an OWL ontology for quantum mechanics. It seems that OWL provides means to model the main conceptual issues that arise in the theory. Problems arise when we try to express in OWL (and even in OWL 2) mathematical details of the theory. Let us give some examples.

Starting to build the ontology we have encountered a problem with complex numbers which are ubiquitous in standard formulation of quantum mechanics (e.g. probability amplitudes are complex numbers, they also occur in the time-dependent Schrodinger equation). One may try to define complex numbers as a new datatype. However, from the point of view of quantum mechanics it is important that real numbers (float) are subsumed in complex numbers. In order to express the subsumption we consider complex numbers not as a datatype but as a class (*ComplexNumber*). Each individual from the class has two properties *realPart* and *imaginaryPart*.

Another problem is related to the representation of an n-ary relations as classes [6]. Consider the commutator relation presented in figure 1. Assume that we want to have a local range restriction on a property *obtainValue* i.e. we restrict the range to a value 0. A class (a subclass of *CommutatorRelation*) obtained in this way represents a binary relation between individuals belonging to a class *LinearOperator*. In quantum mechanics we say that the two operators *commute*. However, it is impossible in OWL to define an object property equivalent to the above binary relation represented as a class. For the same reason we have problems with a representation of an *orthogonality* of quantum states.

There are many places in the ontology where classes (and relations between them) are defined mathematically. Let us consider a class of linear operators (*LinearOperator*). The definition of a linear operator is very simple. However, OWL does not provide means to specify it. In these cases mathematical definitions are included as comments.

5 Conclusion

In this paper, we have presented an OWL ontology for quantum mechanics. The current version of the ontology covers only a small part of actual paradigm of quantum mechanics. We plan to develop the ontology to a more complete form which will be useful for applications.

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