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THE SEMANTIC WEB AND THE ONTOLOGY FOR QUANTUM MECHANICS

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Abstract

Motivations for development of an ontology for quantum mechanics and probable advantages of its using are presented in short.

1 Introduction

The Internet is used by physicists (and in general by scientists) since its beginning. It is worth noticing that World Wide Web was developed in 1989 by Tim Berners-Lee when he was a software engineer at CERN (European Particle Physics Laboratory). At the beginning the system was intended for sharing information within international working groups. Later on new possibilities appeared i.e. the possibility of sending the electronic version of articles to journals and publishing on websites results of research. Special e-print archives have come into being which offer the possibility of placing the electronic versions of articles. The most popular is *http://arXiv.org* archive on which it is possible to place and retrieve articles on physics, mathematics, computer science and biology. The most important advantage of such archives is the collection a lot of papers in one place. It facilitates the scientists to follow the development of their scientific field. Moreover the existence of such archives makes it possible to build the indexes of citations between publications [1]. One can easily establish what paper cites other earlier papers. Indexes of citations enables citation analysis and are used for studies involving research evaluation [2]. However, searching for information stored in such digital archives is rather unsatisfactory mainly because this is a usually syntactic searching. The presence of the word in some paper does not mean that the paper concerns an interesting field for us (e.g. the word may appear in different contexts). We will find out about this after reading the abstract or looking through the paper. This is obviously a time-consuming occupation taking in the account that only in the field of quantum mechanics a dozen articles are added to the database every day. One may ask the question: is it possible to improve access to information and its analysis in the case of repositories and databases of scientific papers? It seems that such a possibility offers the Semantic Web.

2 Syntactic and Semantic Web

Currently most of the information on the Web is intended for human processing (reading). The information is comprehensible only for men and not for machines. Search engines help us to find information, however, it often happens that they return unwanted results.

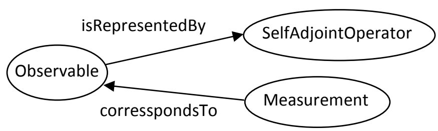
Moreover they may also miss the important information. The existing search-tools are insufficient because they are based on syntactic searching. Hence, the idea of the Semantic Web appeared [3]. The main aim of the Semantic Web is to make the information on the World Wide Web more accessible to machines. The information will be transformed in such a manner that it could be analyzed and processed by machines. The key role in the Semantic Web is played by ontologies. The ontology is the term which originates from philosophy. In that context the ontology is the theory of being and existence i.e. ontology concerns the kinds of things that exists and relationships between existing objects. In computer science the term is used in a similar context i.e. it defines a common vocabulary for sharing information. There exists a variety of ontologies connected with many domains (see e.g.[4]). The search engines will look for pages that refer to a precise concept in an ontology instead of collecting all pages in which certain, generally ambiguous, keywords occur [5]. In this way results of searching will be better fit to queries. To reach this we will require ontologies connected with different domains of knowledge e.g. ontology for quantum mechanics (QM). Existence of such ontology will offer new possibilities. Each paper concerning QM will be analyzed not only from the viewpoint of citations but also from its content view. It is worth noticing that there is a similarity between the current (syntactic) Web and the structure of citations, namely citation links are nothing more than hyperlinks between Web pages. One paper in the bibliography refers to another that may be in (different) archives and similarly one Web page refers to another page. There is no distinction between the references, and similarly there is no distinction between links in the Syntactic Web. The knowledge gathered in archives such as *http://arXiv.org* is not machine interpretable and similarly the knowledge gathered in syntactic Web pages. In order to change the situation and to make the knowledge of QM available for machines we need the ontology for Quantum Mechanics.

3 The ontology for Quantum Mechanics

In the field of Philosophy the ontology is the theory of being and existence. It concerns the kinds of things that exists and relationship between existing objects. Quantum Mechanics is the most fundamental theory of reality. That is why one may try to build the ontology which takes into account the results of the theory i.e. quantum ontology (see e.g. [6, 7, 8]).

Definition

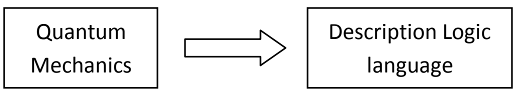
In this paper we are going to consider the ontology for quantum mechanics not in the sense of philosophy but in the sense of informatics. Our aim is to build the ontology which can be useful in the Semantic Web. According to the classical definition of Gruber [9] an ontology is an explicit specification of a conceptualization. A conceptualization is the actual interpretation of a specific domain by a number of humans, which is basically an opinion about the important concepts and their relations. The specification contains precise definitions of the concepts and the relations between them and is usually represented in some ontology language. Common languages to represent ontologies are RDF(S) [10] or OWL [11]. Each language offers different modeling primitives and, thus, a different level of complexity. The question is whether it is possible to build such ontology for quantum mechanics. We assume that it is possible. It seems reasonable to state that quantum mechanics (and in fact each physical theory) can be treated as a set of concepts and a set of relations between concepts. For instance, in quantum mechanics we may consider concepts: the observable, the self-adjoint operator, the measurement. Quantum mechanics fixes the following relations between the concepts: any observable is represented by a self-adjoint operator, with each observable there correspond a measurement i.e. a sequence of physical operations. Hence in the ontology we define above concepts (Observable, SelfAdjointOperator, Measurement) and relations (isRepresentedBy, corresspondsTo). Graphical representation is the following:



Moreover, the ontology may include more sophisticated information such as:

- subclass relationship e.g. class Hamiltonian is subclass of another class Observable,
- disjointness statement e.g. classes Observable and State are disjoint,
- value restrictions e.g. only members of the class Hamiltonian can generate TimeEvolution,
- specification of logical relationship between concepts e.g. probability amplitude is computed for exactly two states.

Quantum mechanics is a discipline that has been developed since the beginning of the last century. We have to define a lot of such concepts and relations. Hence we obtain a conceptualization of the quantum mechanics. The conceptualization have to be written in an appropriate language which allows to represent the knowledge. The most appropriate languages of this kind are languages based on Description Logic (DL)[12]. DL languages are fragments of the first-order predicate logic. One of the most important characteristics of these languages is that they are equipped with a formal, logic-based semantics. Moreover, the languages support reasoning allowing one to derive new knowledge which is implicit in existing descriptions. From this point of view the ontology for quantum mechanics can be seen as an effect of projection of some empirical theory (quantum mechanics) to an appropriate description logic language.



Remarks on quantum mechanics

In order to obtain the above projection (QM to DL) one may try to "reduce" QM to quantum logic [13] and then look for a representation of quantum logic in some DL language[1]. The approach has some advantages e.g. in this way the problem with the ontology of quantum mechanics seems to be placed on a logical level. We must remember however that we want to represent the knowledge of quantum mechanics in the ontology and the ontology must to be useful in searching repositories and databases of scientific papers on quantum mechanics. That is why the ontology should contain all concepts and relations which are meaningful in quantum mechanics and not only in quantum logic which can be seen as a set of rules for reasoning about propositions which takes the principles of quantum mechanics into account. The ontology will obviously contain concepts and relations coming from quantum logic. But not only.

Remarks on Description Logic

The languages based on DL are distinguished by the constructors they provide [12]. The more constructors in the language the more expressive power of the language. And the more expressive power of the language is, the more inefficient the reasoning support becomes. It may happen that the price for the large expressive power will be noncomputability of the language. The question arises which constructors are necessary in the DL language representing the knowledge of QM. It may happen that in order to build the ontology for QM an expressive power is needed beyond any decidable fragment. We will be able to give a complete answer to the question when we have the complete ontology of QM.

Logical consistence

The logical consistency means that the ontology does not contain contradicting information[2]. In science (and in particular in QM) it may happen, however, that results obtained by two scientists are in

[1] Quantum logic can be seen as a fragment of Independence-Friendly Logic (see Hintikka J., Journal of Philosophical Logic, Volume 31, Number 3, June 2002, p. 197) which aims to be a more natural and intuitive alternative to classical first-order logic.

[2] There are also another notions of consistency, see P. Haase and L. Stojanovic, *Consistent evolution of OWL ontologies*, in Proceedings of the Second European Semantic Web Conference, Heraklion, Greece, 2005, MAY 2005.

contradiction. The contradiction is usually easily eliminated. There are, however, situations where the contradiction becomes an element of our knowledge (or unknowledge?) for a long time. This may result in nonconsistence of an appropriate ontology. And this has an obvious influence on the reasoning because conclusions drawn from an inconsistent ontology may be completely meaningful. Nevertheless there exists a framework which support reasoning with inconsistent ontologies [15].

Other ontologies

Finally it is worth pointing out that due to a crucial role played in Quantum Mechanics by mathematics (in fact the theory can be seen as an interpreted mathematical structures) the ontology will use purely mathematical concepts (e.g. selfAdjointOperator). Moreover, quantum mechanics is a part of physics, hence, the ontology for QM will also use entities from physics (e.g. physical quantity). It seems reasonable that the ontology for quantum mechanics will use concepts and relations from ontologies of mathematics and physics.

4 quONTOm

A preliminary and rather a simple version of the ontology for QM named *quONTOm* is available on:

http://merlin.fic.uni.lodz.pl/quONTOm

Due to a highly complicated field this ontology is at the moment incomplete and it will be gradually developed towards a more complete form. The ontology is written using Protégé ontology editor [14] and OWL-DL sublanguage which permits efficient reasoning support[3]. Actually *quONTOm* ontology in practice is contained in one OWL document. The document contains also entities (classes, properties etc.) which are not parts of QM ontology (e.g. purely mathematical objects). In the prepared, new version of the ontology the elements will be separated from *quONTOm* and will become parts of auxiliary ontologies (e.g. mathematics, physics and others).

[3]DL expressivity of *quONTOm* is *SHOIN(D)*

5 Future perspective

Despite the fact that the ontology for quantum mechanics is not constructed yet we may formulate some future perspectives. At present the knowledge of QM is contained in books and in human minds. The ontology for QM makes it possible to represent the knowledge in the machine processable and interpretable language. Such possibility will offer new advantages. First of all searching for and the exchange of the information about QM between scientists can be more effective. The ontology for QM will can be used in description of experiments (and obtained results). Thanks this an automatic processing of experimental data will be possible. This in turn will make possible the execution of queries concerning conducted experiment possible. This will be probably possible in the near future. However, we may go further. Nowadays reporting any scientific result in QM (and not only) involves writing a paper at least in the electronic version. Maybe in the future the reporting will also (only?) consist of introducing a change to the ontology corresponding with QM. Considering results of the research as a set of changes in the ontology will allow to evaluate the importance of the changes and research. It will be possible to introduce measures of changes introduced in the ontology. And this makes possible to execute queries such as "Retrieve all authors that changed the ontology for QM most of all in the last three years". The result may differ from the result of the query "Retrieve all authors that have the most papers on quantum mechanics in the last three years". And even if the machines will not be able to extend our knowledge they at least will be able to check whether our knowledge is consistent e.g. whether the results published in one article are not in contradiction with already published results. This situation will result in an inconsistency in the ontology. Thanks to use of machines we will be informed about this.

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