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A Case Study of Ontology Evolution in Atomic Physics as the Basis of the Open Structure Ontology Repair Plan*

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Abstract

In the GALILEO project a number of *Ontology Repair Plans* are being developed and implemented in higher-order logic. These plans resolve a contradiction between two or more ontologies that represent the domain of physics. In this abstract, the transition from Thomson's *plum pudding model* of the atom to Rutherford's *planetary model* is used as the main inspiration of a new ontology repair plan called *Open Structure*

1 Introduction

In the framework of the GALILEO project (Guided Analysis of Logical Inconsistencies Leads to Evolved Ontologies) a number of *Ontology Repair Plans* (ORPs) are being developed and implemented in higher-order logic. For reasons of space, the interested reader is referred to [Bundy and Chan, 2008] to find general indications on how the overall GALILEO approach, and thus what presented in this abstract, relates to analogues in the literature. It should be noted, though, that GALILEO's future research objectives do include a more precise positioning of the notion of ORP with respect to existing formal-ontological and epistemological approaches. ORPs resolve a contradiction between two or more ontologies that represent the domain of physics. In ORPs developed thus far, one of the ontologies represents a physical theory – its theorems are interpreted as expectations or predictions; a second ontology represents a sensory or experimental set-up for that theory – its theorems are interpreted as observations. When the sensory ontology generates a theorem that contradicts a theorem of the theoretical ontology – i.e., when an observation contradicts an expectation – an ORP kicks in and amends the two ontologies. Such repair enables the theoretical ontology to make correct predictions and updates the experimental ontology with the new theory. ORPs may act either as theory revision mechanisms or as signature revision mechanisms – in the latter case they bring about an evolution of the ontologies by changing their representation language.

The development of ORPs is inspired by cases in the history of physics where the transition from an old theory to a new one was forced by a contradiction between observations and predictions. For instance, the discovery of Latent Heat inspired the ORP called *Where is my stuff?* (WMS). This plan changes the signature of the ontologies by splitting a function into a *visible* and an *invisible* part; such repair accounts for the impossibility, at a given moment of the history of physics, to fully measure a given quantity (e.g. heat or presently mass, as Dark Matter has never been measured directly). The transition from Boyle' Law to the Ideal Gas Law inspired the ORP called *Inconstancy*, which changes the signature of the ontologies by adding an argument to a function; it may, for instance, make a constant (e.g. the volume to pressure ratio of a gas) dependent on an quantity (e.g. temperature). The case of the ancient distinction between the Morning Star and the Evening Star, later identified by astronomers as the same planet Venus, inspired the recently proposed ORP called *Unite*. This plan operates as a theory revision mechanism which equates two functions.

The present abstract provides an example of a modeling exercise, from historical analysis to formalization. The transition from Thomson's *plum pudding model* of the atom to Rutherford's *planetary model* is used as source of inspiration of a new ORP called *Open Structure* (OP) and of its inverse, not presented here, called *Close Structure* (CS). OS and CS operate as theory revision mechanisms, which delete one of the cases of a function, thus restructuring a given entity (e.g. an atom) by distributing a given quantity differently (e.g., the work excerted by an atom's positive electric field on a particle orbiting around it)[1]. Section 2 presents part of the historical analysis that led to *Open Structure* and presents the formulae that may be subject to ontological evolution. Section 3 presents *Open Structure* and its application to the case study. Section 4 sets further research objectives.

2 From Thomson's to Rutherford's Atom

Thomson's Atom Around 1904 Thomson believed that the atom was a uniform sphere of positive charge, as represented in Fig. 1 (left), with electrons rotating and oscillating in it. Negative charges were placed on concentric rings or at the

*I'm grateful to Alan Bundy, Michael Chan and the ARCOE-09 reviewers for comments on earlier drafts.

[1] As noted by Alan Bundy during a recent private exchange, in general mathematical terms it may be said that OS and CS let a non-monotonic function evolve into a monotonic one.

center. The number of (electrons on) the rings would increase monotonically while the number of charges at the center would periodically increase and decrease [Baily, 2008].

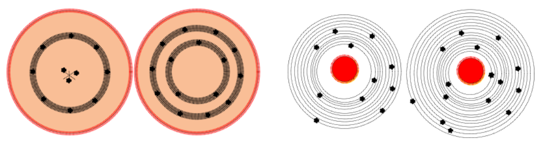

Figure 1: Left: Thomson's atom (11 electron atom and 15 electron atom). Right: Rutherford's atom (11 electron atom 15 electron atom). Black dots and circumferences represent negative charges and their orbits; red circles represent positive charge (more intense where darker).

Scattering Experiment Together with Geiger and Marsden, around 1911 Rutherford learnt how to control a heavy emission named α-particle, i.e. doubly positively charged helium atoms (He2+). Using the apparatus shown in Fig. 2[2], a stream of alpha particles originating from source R was shot at a thin foil of gold atoms (F). Scintillations, which were due to the particles scattering against a rotating screen (S), were observed through a microscope (M) mounted behind the screen. The chamber was evacuated and could be rotated around the foil.

Based on Thomson's model, Rutherford expected the sphere

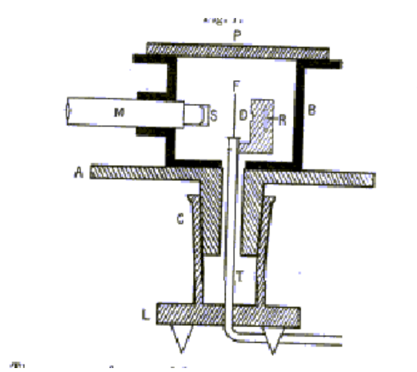

Figure 2: Rutherford's scattering apparatus

of positive charge and the electrons in it to offer virtually no resistance to the passage of α-particles. Given their high speed, their momentum would overcome the repulsion excerted by the positively charged sphere. Thus the particles would be deflected slightly (just like, on left side of Fig. 3, the trajectories with impact parameter around $\pm\, b'$) or go straight through (like virtually all other trajectories). Also, since α-particles are 7000 times heavier than electrons, their trajectory would never be curved by electrons (that is why no negative charges are represented in Fig. 3). Contrary to the expectations, three degrees of scattering were observed:

- most α-particles passed straight through the gold foil *without any or with very little deflection* (like most particles with impact parameters between $\pm\, b$ and $\pm\, b'$ on right side of Fig. 3);
- some α-particles were deflected through *large angles* (i.e. particles with impact paraments around $\pm\, b$);
- a few α-particles *rebounded completely* (i.e. particles with impact parameter around 0).

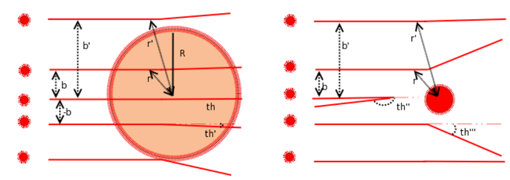

Figure 3: Left: expected scattering. Right: observed scattering. Small red spots represent α-particles; red lines represent particle's paths; half-dashed thin red lines represent ideal undeflected paths; b's and $-b$'s are impact parameters, i.e. perpendicular distances between a particle's velocity vector and the centre of the target atom ($b = 0$ for third particle); r's are distances between a point of the atom's electric field and the atom's center; R is the atom's radius; th's are scattering angles.

Rutherford's Atom Rutherford analyzed the results of the experiment in terms of Newtonian mechanics and obtained a formula to calculate the *differential scattering cross-section* of the α-particles, i.e. the probability, given the impact parameter, of an α-particle to be deflected through a given angle. This made it possible to derive the following conclusions:

1. Since most of the α-particles were not deflected, there is a lot of empty space in an atom.
2. Since some of the α-particles were deflected, there is a centre of positive charge in an atom.
3. Since very few α-particles rebounded, the nucleus is very dense and hard.
4. Since 1 to 3, the structure of an atom is comparable to the Solar System's structure, with the nucleus forming the main mass and the electrons revolving around it.

Evolution between the Two Atoms As shown in [Zoli, 1998], the differences between the scattering of α-particles in Thomson's and Rutherford's atoms may be expressed in various ways. One way is to define two distinct *scattering potential functions* (like 1 below for Thomson and 2 for Rutherford) to calculate the amount of work excerted by the electric fields of the two atoms when deflecting incident particles placed at a distance r from their centers. Note that both potentials are central but, while 1 is both non-Coulombic (i.e. for values of r lower than the atom's radius R, the potential is directly proportional to r) and Coulombic (i.e. for values of r higher than R, the potential is inversely proportional to r),

[2]Originally in [Geiger and Marsden, 1913], downloaded from: galileo.phys.virginia.edu/classes/252/Rutherford_/Scattering/Rutherford_Scattering.html

2 is only Coulombic (R needs not to be considered).

$$V(r)_T = \begin{cases} \frac{Q_A Q_B}{4\pi\epsilon_0}\frac{1}{r} & R \leq r \\ \frac{Q_A Q_B}{4\pi\epsilon_0}\frac{1}{2R^3}(3R^2 - r^2) & 0 \leq r \leq R \end{cases} \quad (1)$$

$$V(r)_R = \frac{Q_A Q_B}{4\pi\epsilon_0}\frac{1}{r} \quad (2)$$

where Q_A is the charge of incident particle, Q_B is the charge of the target atom, $1/4\pi\epsilon_0$ is the Coulomb constant, r is the distance between the incident particle and the centre of the target atom, R is the radius of the target atom.

3 Open Structure Ontology Repair Plan

In this section the evolution from $V(r)_T$ to $V(r)_R$ is modeled by *Open Structure* (3 below). The idea of the plan is to evolve a function that has values that are partly directly proportional and partly inversely proportional to its argument into a function that is only inversely proportional to its argument. In this way the physical structure of the entity described by the function loses an internal and/or external boundary.

Just like all ORPs, OS models the function that is subject to evolution as stuff. V is stuff. Just like V ranges over the type dis of distances r's, stuff ranges over a type δ. The distance R plays the role of cut-off point of V. So stuff's domain contains a cut-off point, *cop*. As the relation between all other quantities in V is constant, these are modeled as K. Two cases of contradiction between O_t and O_s trigger OS:

1. In O_t, for all arguments below the cut-off point, the value of stuff is directly proportional to the argument, while for all other arguments the value of stuff is inversely proportional to the argument. In contrast with this, in O_s the value of stuff is always inversely proportional to its argument. In this case, the solution of the contradiction by OS results in the structure of the entity described by the function to lose a physical internal boundary (where the function is at its maximum).
2. In O_t, for all arguments below the cut-off point, the value of stuff is inversely proportional to the argument while, for all other arguments, the value of stuff is directly proportional to the argument. O_s is the same as in the first case above. Here, after applying OS, the structure of the entity described by the function loses a physical internal boundary (where the function is at its minimum) as well as an external boundary (where the function is at its maximum).

In all cases the contradiction is repaired according to what dictated by O_s (4 through 6 below). This is also true for the inverse of OS, Closed Structure, but here O_s forces the acquisition of an external boundary.

OS may be formlized and applied to the case study as below.

Trigger

$$\begin{aligned} & O_t \vdash d_4 > d_3 \geq cop \geq d_2 > d_1 \wedge \quad (3) \\ & \quad ((\mathit{stuff}(d_2) > \mathit{stuff}(d_1) \wedge \mathit{stuff}(d_3) > \mathit{stuff}(d_4)) \vee \\ & \quad (\mathit{stuff}(d_1) > \mathit{stuff}(d_2) \wedge \mathit{stuff}(d_4) > \mathit{stuff}(d_3))). \\ & O_s \vdash \forall d, d' : \delta.\ d' > d \rightarrow \mathit{stuff}(d) > \mathit{stuff}(d'). \end{aligned}$$

Open Structure

$$\nu(\mathit{stuff}) ::= \lambda d : \delta.\ K/d. \quad (4)$$

Create New Axioms

$$\begin{aligned} & Ax(\nu(O_t)) ::= Ax(O_t) \setminus \quad (5) \\ & \quad \{\mathit{stuff} ::= \lambda d : \delta.\ (cop > d \wedge Kd) \vee K/d\} \cup \\ & \quad \{\nu(\mathit{stuff}) ::= \lambda d : \delta.\ K/d\}. \\ & Ax(\nu(O_s)) ::= Ax(O_s) \setminus \quad (6) \\ & \quad \{\mathit{stuff} ::= \lambda cop, d : \delta.\ (cop > d \wedge Kd) \vee K/d\} \cup \\ & \quad \{\nu(\mathit{stuff}) ::= \lambda d : \delta.\ K/d\}. \end{aligned}$$

The following substitutions in the atom case study would yield the repair below:

$$\left\{ V/\mathit{stuff}, d_i/r_i, cop/R, K/\frac{Q_A Q_B}{4\pi\epsilon_0} \right\}$$

$$\begin{aligned} & Ax(\nu(O_t)) ::= Ax(O_t) \setminus \\ & \quad \{V ::= \lambda r : dis.\ (R > r \wedge Kr) \vee K/r\} \cup \\ & \quad \{\nu(V) ::= \lambda r : dis.\ K/r\}. \\ & Ax(\nu(O_s)) ::= Ax(O_s) \setminus \\ & \quad \{V ::= \lambda r : dis.\ (R > r \wedge Kr) \vee K/r\} \cup \\ & \quad \{\nu(V) ::= \lambda r : dis.\ K/r\}. \end{aligned}$$

4 Conclusion

The transition from Thomson's *plum pudding model* of the atom to Rutherford's *planetary model* was used as the basis of a new ontology repair plan called *Open Structure* and of its inverse, *Close Structure*. Future research will focus on:

- the interpretation of the second case of OS: what are the examples of the physical structure represented by O_t in the OS's second case?;
- the interpretation of CS, OS's inverse: what are the examples of the physical structure represented by O_s in CS?
- the alternative to OS and CS: what would be the advantages of modeling the evolution between the two atoms in terms of their different scattering angle functions (i.e. by comparing alternative trajectories of particles that have the same impact paramater)?

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