

# Open Structure: Ontology Repair Plan based on Atomic Modeling

Jos Lehmann

joint work with Alan Bundy and Michael Chan

School of Informatics, University of Edinburgh

ARCOE 2009



# Outline

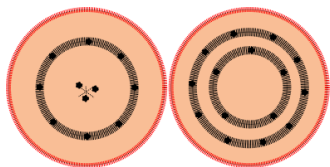
- 1 Overview GALILEO Project
  - Ontology Evolution in Physics
- 2 A Case Study in Atomic Modeling
  - From Thomson's to Rutherford's atom
- 3 Ontology Repair Plan based on Case Study
  - Open Structure
- 4 Discussion
  - Future work



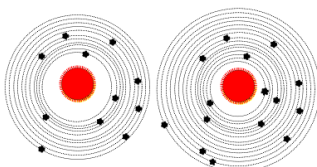
# GALILEO project and Ontology Evolution in Physics

- Aim: solving contradictions between multiple ontologies.
  - Canonical case: contradictions in physics between theoretical expectations and experimental observations.
- Main results: Ontology Repair Plans (ORPs).
  - Trigger: detects contradiction between ontologies.
  - Repair: changes ontology axioms or signature.
  - Create New Axioms: propagates changes as needed.
- Methodology: turn case studies in physics history into ORPs.
  - Extract ORP's conceptual backbone from case study.
  - Represent ORP in higher-order logic.
  - Implement ORP ( $\lambda$ Prolog and beyond).
- Some ORPs and their state of development.
  - Developed and tested: Where's My Stuff?, Inconstancy, Unite.
  - Being tested: Open Structure, Close Structure.
  - Under development: Unify.

# Thomson's atom (1904) and Rutherford's atom (1911)



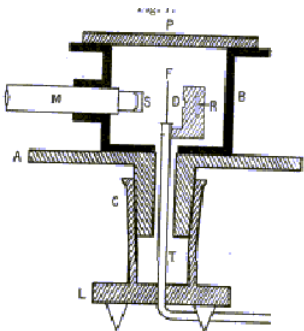
Thomson's Atom



Rutherford's Atom

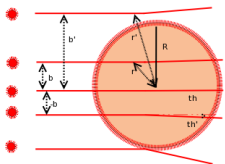
- 11 electron atom and 15 electron atom.
- Black dots and circumferences represent negative charges and their orbits/rings.
- Red circles represent positive charge (more intense where darker).
- Note that Rutherford's atom's structure is monotonic: Thomson's atom's configuration changes when electrons are added, Rutherford's atom's configuration is stable.

# Rutherford's scattering apparatus (1898-1911)

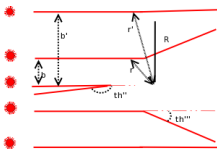


- R, fixed source of  $\alpha$ -particles (double positive charges).
- D, collimating diaphragm.
- F, fixed foil.
- S, screen.
- M, microscope.
- Chamber is evacuated and can be rotated around F.
- Original image in (Geiger, 1913), downloaded from. <http://galileo.phys.virginia.edu>

# Expected vs observed scattering



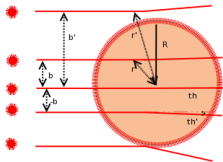
Expected Scattering



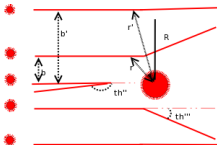
Observed Scattering

- Red spots and lines are  $\alpha$ -particles and their paths.
- Half-dashed thin red lines are ideal undeflected paths.
- $b$ 's and  $-b$ 's are impact parameters ( $b = 0$  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.
- **Expected scattering is minimal.**
- **Observed scattering is minimal, large or a complete rebound.**

# The nucleus



Expected Scattering



Observed Scattering

- The nucleus explains the difference between expectations and observations.
- The nucleus entails different *deflection functions*:

$\theta(b)_{Thomson}$  and  $\theta(b)_{Rutherford}$  calculate different deflection angles for same  $b$ 's.

- The nucleus also entails different *scattering potential functions*:

$V(r)_{Thomson}$  and  $V(r)_{Rutherford}$  calculate different amounts of work exerted by positive electric fields when deflecting incident particles at same distance  $r$ .

# Scattering potential functions for different structures

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

$$V(r)_{Rutherford} = \frac{Q_A Q_B}{4\pi\epsilon_0} \frac{1}{r}$$

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.

- $V(r)_{Thomson}$  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  $r$ ).
- $V(r)_{Rutherford}$  is only Coulombic ( $R$  needs not to be considered).
- Formulae taken from (Zoli, 1998)





# Evolution of $V(r)$ by existing ORPs

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

$$V(r)_{Rutherford} = \frac{Q_A Q_B}{4\pi\epsilon_0} \frac{1}{r}$$

- **Where is my stuff?** would stick to Thomson's atomic structure by increasing  $Q_A$  and yielding evolution  $V(r) ::= V(r)_{vis} + V(r)_{invis}$ . Problem: how would the additional charge be distributed wrt  $R$ ?
- **Unite**, the inverse of Where is my stuff?, would not be able to let  $V(r)$  evolve.
- **Incons** too would stick to Thomson's atomic structure and let  $V(r)$  evolve in such a way that the Coulomb constant  $1/4\pi\epsilon_0$  would depend on distance  $r$  from the center of atom. This would yield a very complicated structure.
- **Need for an ORP that handles structural evolution as such**, rather than by pivoting on quantities.
- Formulae taken from (Zoli, 1998)



# Open Structure ORP: Trigger

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

- *stuff* represents function subject to evolution ( $V$  is *stuff*).
- *stuff* ranges over a type  $\delta$  of  $d$ 's (like  $V$  ranges over the type *dis* of distances  $r$ 's).
- *stuff*'s domain contains a cut-off point *cop* (like  $V$ 's domain contains  $R$ ).
- $K$  is constant (like all other quantities remain constant throughout  $V$ 's evolution).
- Two cases of contradiction:

**crested\* vs open structure** In  $O_t$ , for all arguments below cut-off point, value of *stuff* is directly proportional to argument, inversely proportional otherwise. In  $O_s$  value of *stuff* is always inversely proportional to argument.

**trenched\* vs open structure** In  $O_t$ , for all arguments below cut-off point, value of *stuff* is inversely proportional to the argument while, directly proportional otherwise.  $O_s$  is the same as in the first case above.

\*tentative term



# Open Structure ORP: Repair & Create New Axioms

**Open Structure** :  $\nu(stuff) ::= \lambda d : \delta. K/d.$

**Create New Axioms** :  $Ax(\nu(O_t)) ::= Ax(O_t) \setminus$

$\{stuff ::= \lambda d : \delta. (cop > d \wedge Kd) \vee K/d\} \cup$

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

$Ax(\nu(O_s)) ::= Ax(O_s) \setminus$

$\{stuff ::= \lambda cop, d : \delta. (cop > d \wedge Kd) \vee K/d\} \cup$

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

- Contradiction always repaired according to what dictated by  $O_s$ .

# Application of Open Structure

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

$$\begin{aligned} \text{Trigger : } O_t \vdash r_4 > r_3 \geq R \geq r_2 > r_1 \wedge \\ & ((V(r_2) > V(r_1) \wedge V(r_3) > V(r_4)) \\ O_s \vdash \forall r, r' : \text{dis. } r' > r \rightarrow V(r) > V(r'). \end{aligned}$$

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

# Future work

- Find other cases for application of Open Structure.
- Interpret its inverse, Close Structure, and find cases of application.
- Alternative treatment of Thomson vs Rutherford case study: modeling the evolution between the two atoms in terms of their different deflection functions.

