Theories and models: an approach from quantum chemistry

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Aims of the presentation

General Objective:

- To establish that the independence of models from theories allows to advocate for an instrumentalist point of view of theories.

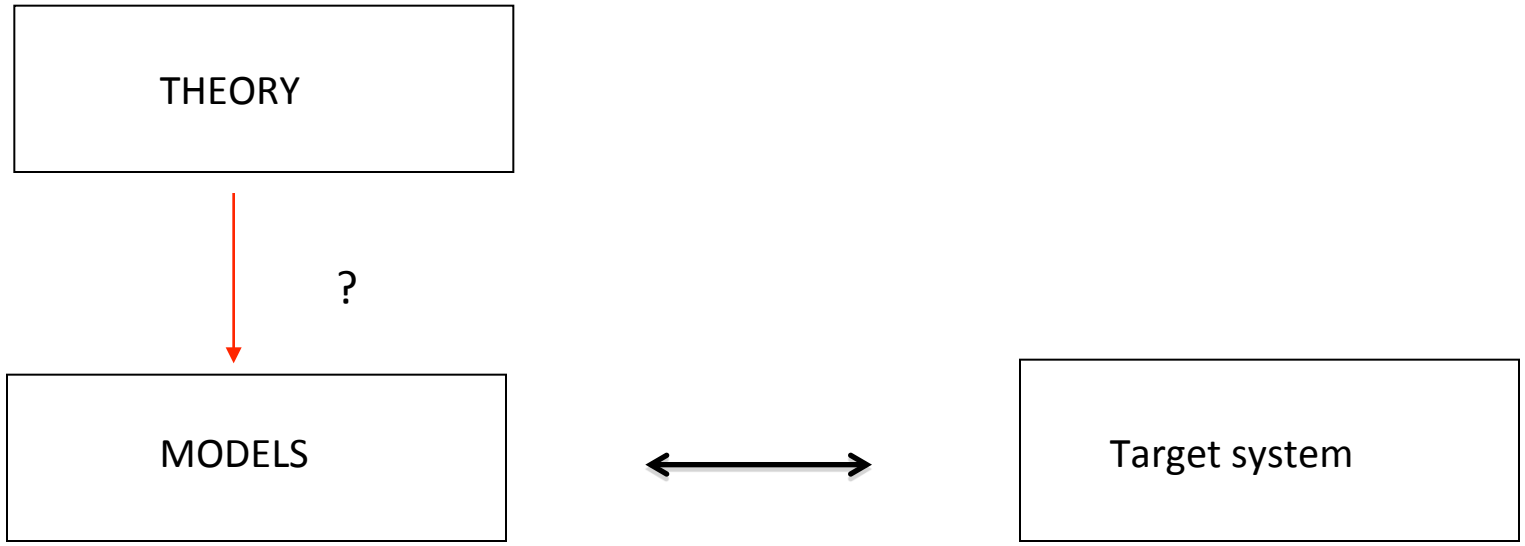
Specific objectives:

1. To summarize the fundamental theses of **the theory-driven conception** supported by the Semantic View

2. To analyze the discussions around the **London brothers´ model of superconductivity**. Our aim is to show that the debate has reached a dead end as a consequence of some disagreements with the interpretation of the notion of independence and its role in the constitution of scientific models.

3. We intend to overcome the dead end by appealing to a new example: the case of the **molecular models used in quantum chemistry**. It will provide an argument in favour of the independence of models

Why does this issue matter ?



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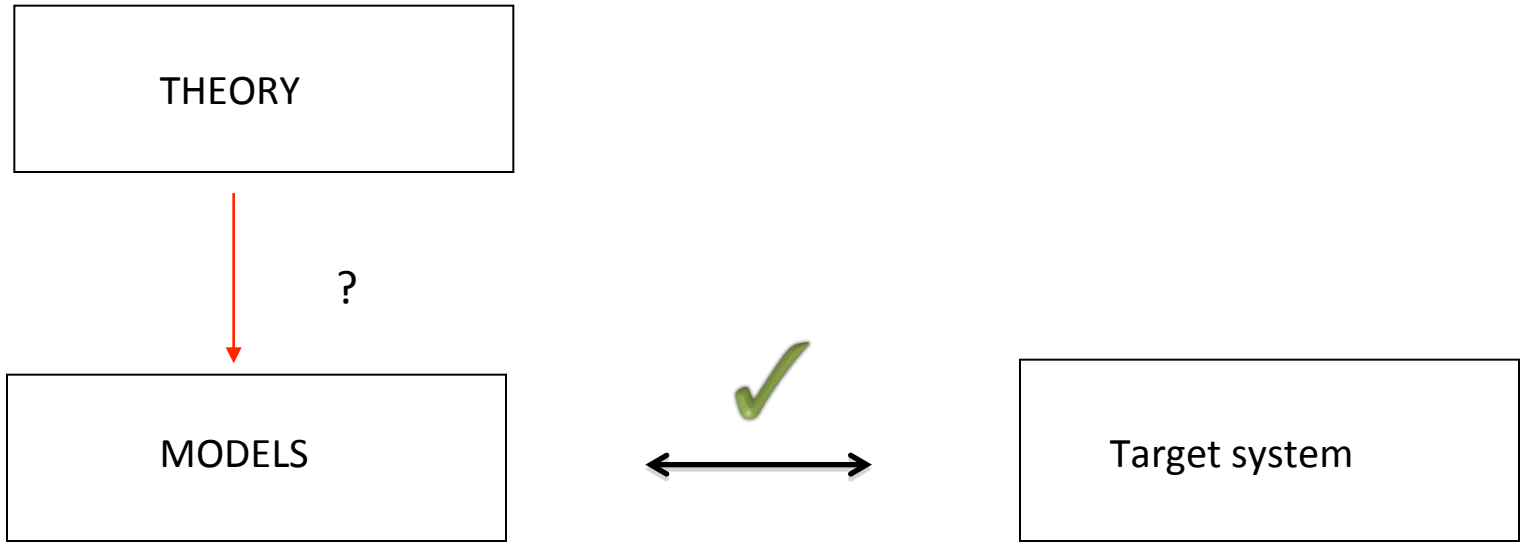

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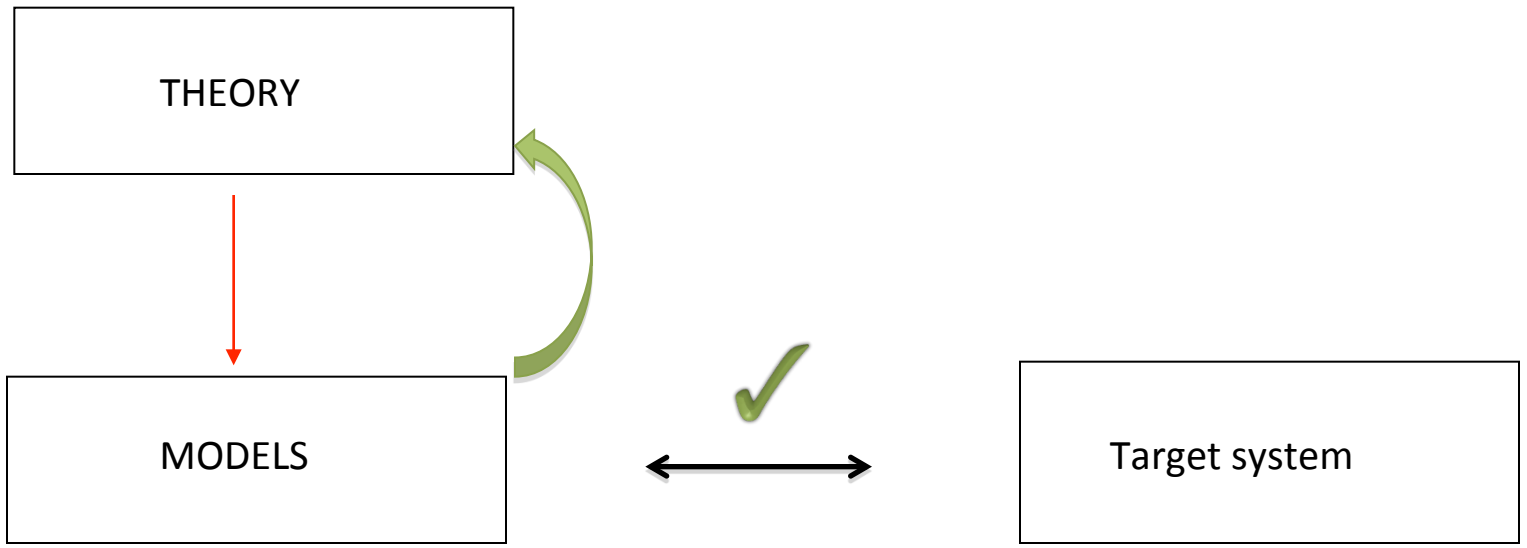

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1. Theory-driven point of view

The Semantic View:

- Theories are not a collection of propositions but extra- linguistic entities.

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A theory is presented through its sets of models

↓

A theory contains in a relevant way all its models

1. Theory-driven point of view

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- ✓ Models must be models *of* theories because they are their truth-makers.

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Inconsistent with Ohm´s law (I = E/R): I remains without E.

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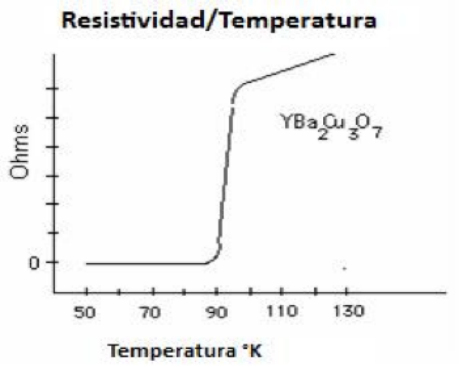

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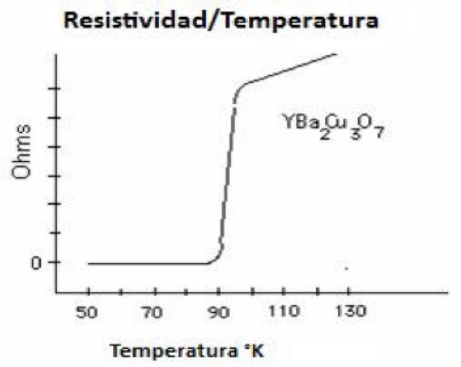

3- **Same crystal structure**

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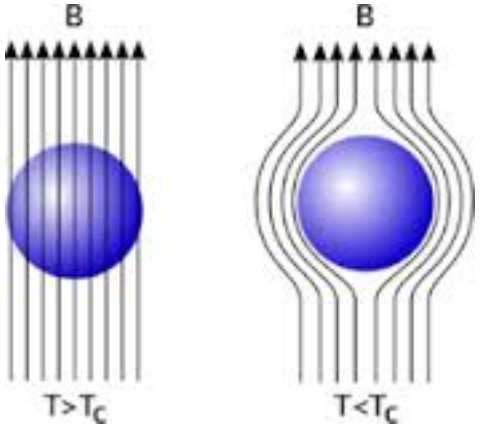
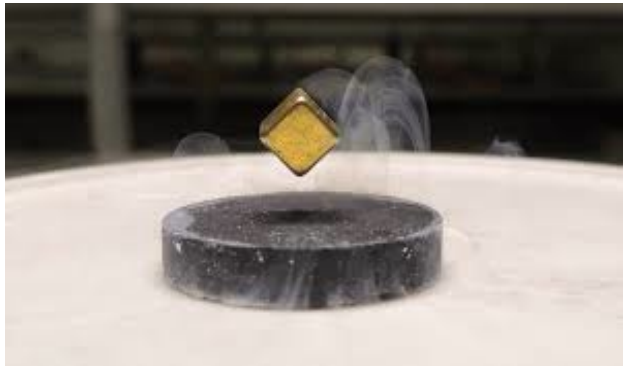
3- **Meissner effect**: when superconducting materials reach the critical temperature in presence of magnetic field, they expel all the electromagnetic flux. ($B_{int} = 0$)





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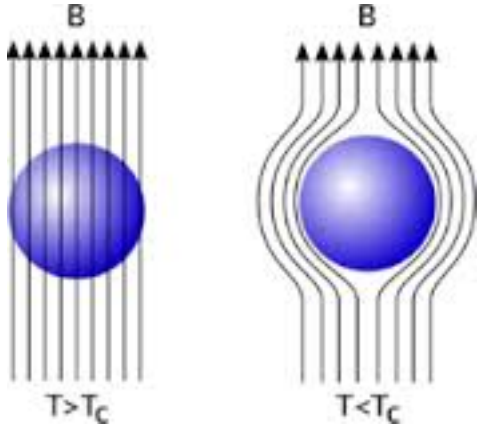

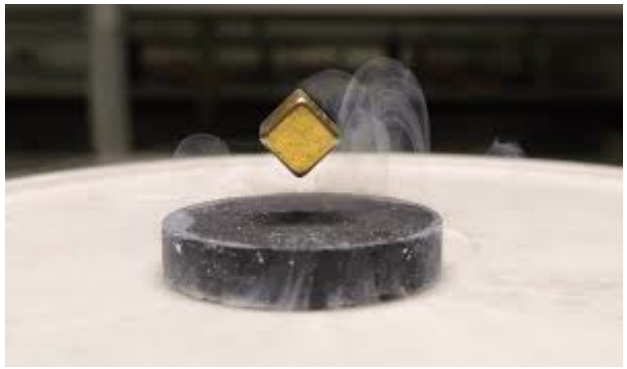

In spite of having the same structure the <u>Meissner effect is inconsistent with the Maxwell´s equations</u>

↓

Faraday´s law (rot E = −dB/dt) predicts that when E → 0, it must be that − dB/dt = 0 and so the magnetic field B must remain constant B.

2. Superconductivity: *the London brothers' model (1935)*

$$\nabla^2 B = \lambda_L^{-2} B$$

$\nabla^2 B$ → Magnetic field

λ_L^{-2} → the London penetration depth

They could calculate the distance at which a magnetic field penetrates into a superconductor

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Analyzing the model: two points of view

I. The so called *Toolbox View of Theories* (M. Suárez, N. Cartwright, T. Shomar)

II. The revisionists of The Semantic View (S. French, J. Ladyman, O. Bueno, N da Costa)

2. Superconductivity: *the London brothers' model (1935)*

The core of the debate

How was the London brother´s model built?

↓

Does the model contradict the **theory – driven** thesis of the Semantic View?

- ***Toolbox* : Yes**, it does
- ***Revisionists***: **No**, it does not

The Toolbox View of Theories

The London model:

The Meissner effect cannot obtain given Ohm ´s law and the acceleration equation

M.Suárez & N.Cartwright

"Yet, we want to retain the consequences of the acceleration-equation model for resistanceless flow. The London model manages to have its cake and eat it too.
But there was nothing in the theory that legitimates using Ohm´s law for some materials while holding it in abeyance for those that turn out to be superconducting" (p. 65, 2008)

The Toolbox View of Theories

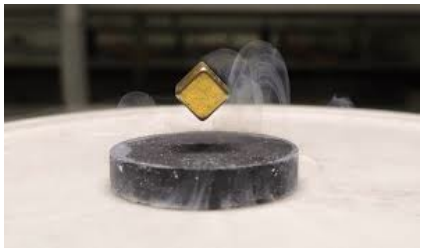
Theory-driven:

ELECTROMAGNETIC THEORY CURRENT IN 1933

Legitimate the modification of

$$\nabla^2 B = \lambda_L^{-2} B$$

Confirms



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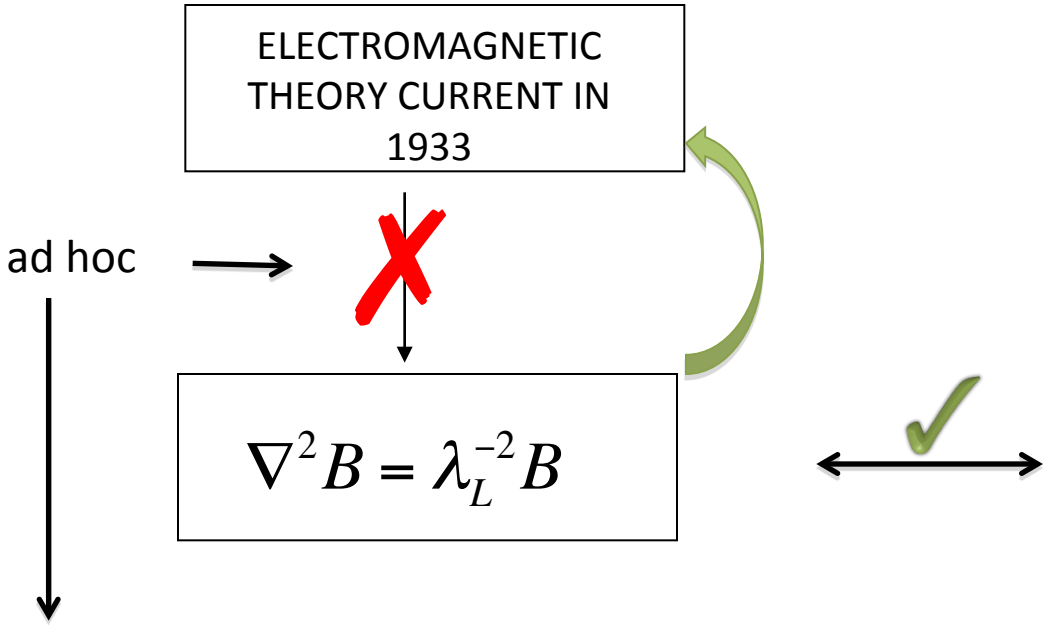

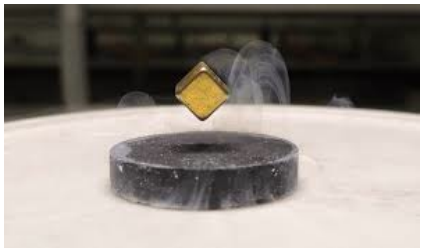

The London model was not produced by a de-idealization: **the analogy with diamagnetism was not possible before the discovery of the Meissner effect and it was not legitimated by the Electromagnetic Theory of 1933.**

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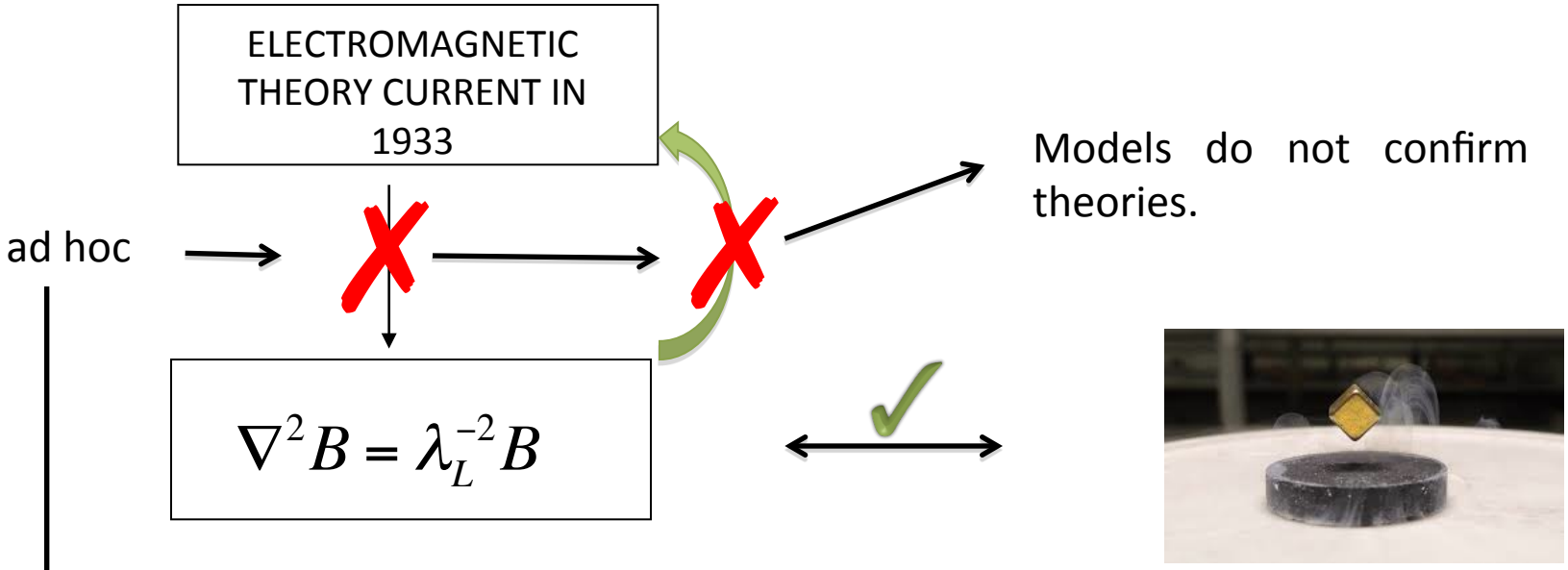

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- London Model is independent from the theory
- Theories are just instruments that together with other things are used to build them

The revisionist of The Semantic View

- The disagreements are not about technical details
  - Both accepted that the analogy with diamagnetism was not legitimated by the Electromagnetic Theory.
  - Both accepted that the model could not be possible without the Meisnner effect

Da Costa & French

"The model may be functionally independent (…) **but they are not so independent from all theory**" (p124. 2000)

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It is relative and historical

It seems that they interpreted that the toolbox means that theories play no role

The misunderstanding of the notion of independence

1. We should not identify dependence with deduction and independence with not deduction ✗

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Suárez & Cartwright

"Of course, we agree that the broad theoretical context is provided by Maxwell´s equation- this was our starting point" (p.70)

"This notion of `independent´ is of course historical, and hence the autonomy that grounds it may well be only temporary" (p.68)

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↳ **Toolbox View:**

- Theories are instruments useful to construct models
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The paradigmatic example is useful neither to determine nor to undermine the theory-driven point of view.

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3. Molecular models in quantum chemistry

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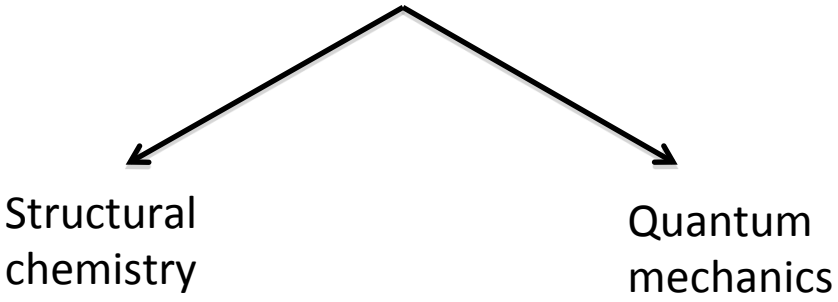

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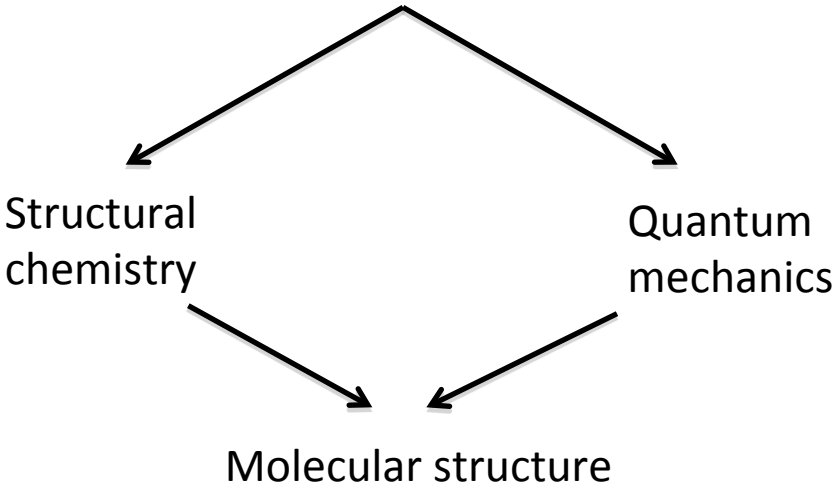

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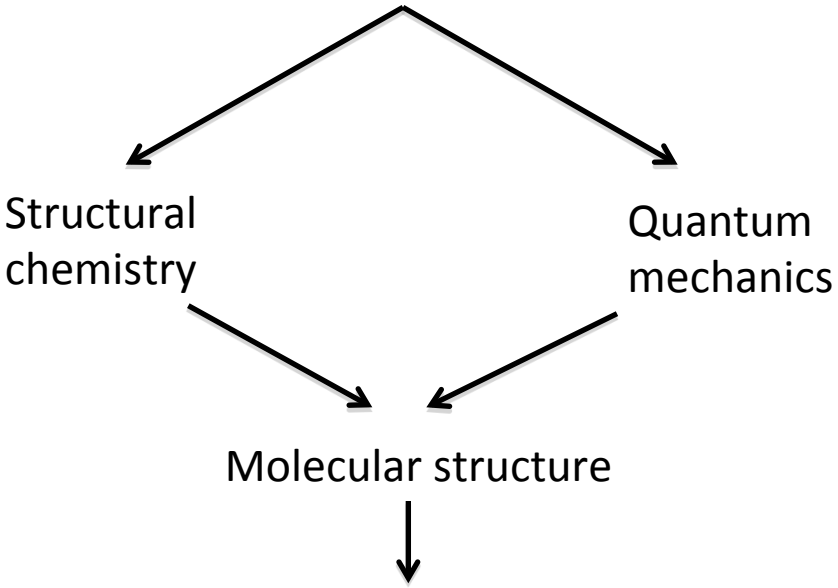
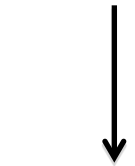


- **"**Molecular structure is so central to chemical explanation that to explain molecular structure is pretty much to explain the whole of chemistry**"** (Hendry 2010, p. 183)
- "Is the central dogma of molecular science" (Woolley 1978,p.1074)

↓

Chemistry works on the basis of the energy of the system

Using quantum mechanics to determine molecular structure



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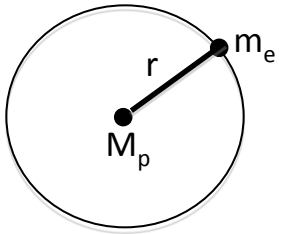

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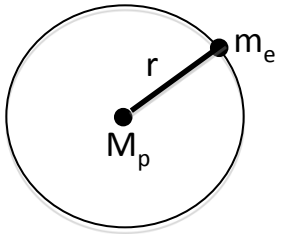
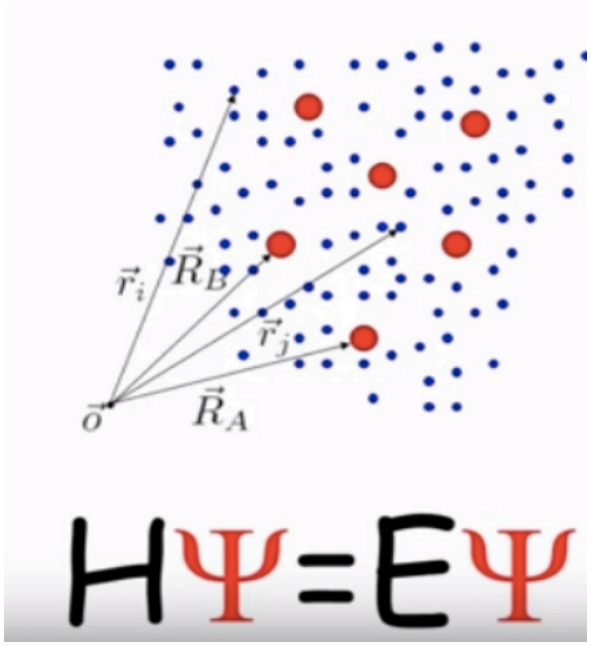


$$H_{tot} = \frac{p_N^2}{2M} + \frac{p_e^2}{2m_e} - \frac{e^2}{|R_N - r_e|}$$

- $\frac{p_N^2}{2M}$: Kinetic energy of the nucleous
- $\frac{p_e^2}{2m_e}$: Kinetic energy of the electron
- $\frac{e^2}{|R_N - r_e|}$: Electrostatic interaction between the electron and the nucleous

These are all the interactions of the system

Polynuclear System



$$H_{tot} = \sum_{\alpha} \frac{p_{\alpha}^2}{2M_{\alpha}} + e^2 \sum_{\alpha<\beta} \frac{Z_{\alpha} Z_{\beta}}{|R_{\alpha} - R_{\beta}|} + \sum_{i} \frac{p_i^2}{2m_e} - e^2 \sum_{i} \sum_{\alpha} \frac{Z_{\alpha}}{|r_i - R_{\beta}|} + e^2 \sum_{i<j} \frac{1}{|r_i - r_j|}$$

- Kinetic energy of the nuclei
- Electroestatic interaction between the nuclei
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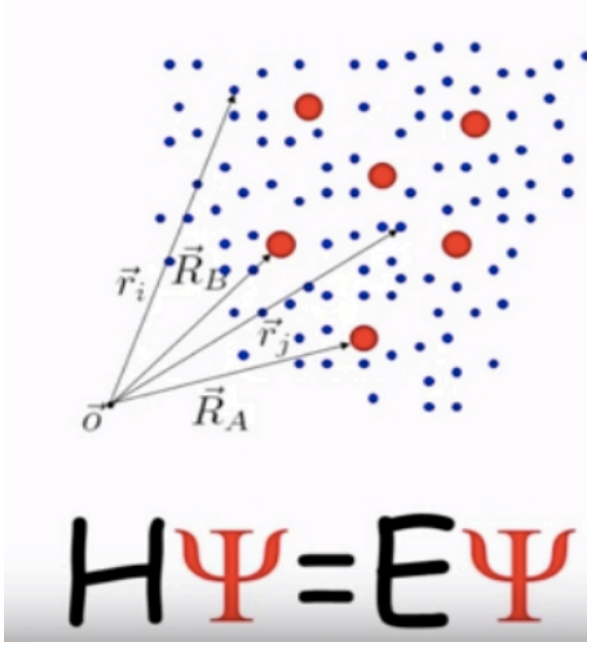

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- $\sum_{i} \frac{p_i^2}{2m_e}$: Kinetic energy of the electrons
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It does not have any analytical solution

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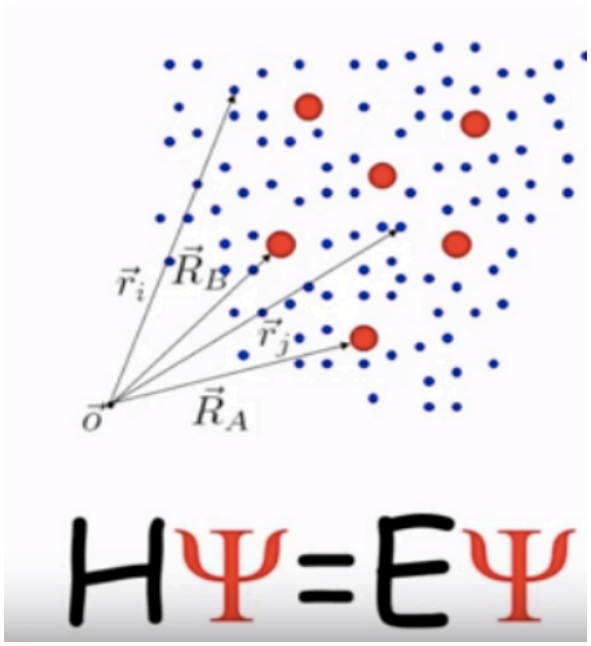

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To solve the hamiltonian for polynuclear system the **Born – Oppenheimer approximation was proposed**

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- By eliminating the kinetic energy, they eliminate the energy generated by the movement and it is assumed that the nuclei are fixed → *clamped nuclei approximation*

The critical step is justified by assuming that $M_\alpha >> m_e$. So, in the limit case $m_e/M_\alpha \rightarrow 0$ and kinetic energy tend to 0

This defined values of position and of momentum (0)

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This is incompatible with Heisenberg's *principle of uncertainty* according to which quantum particles cannot simultaneously have well defined position and momentum

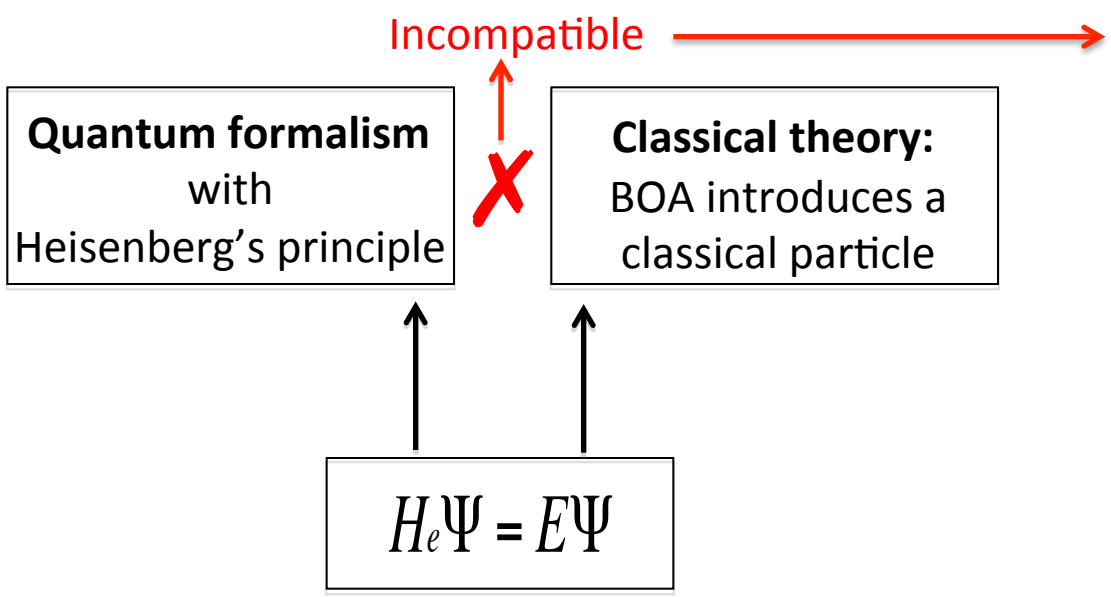
Rejecting the theory-driven point of view

Quantum formalism
with
Heisenberg's principle

Classical theory:
BOA introduces a
classical particle

$$H_e\Psi = E\Psi$$

Rejecting the theory-driven point of view



"This picture is non-quantum in a very fundamental way as the simultaneous assignment of fixed positions and fixed momenta (namely, zero) to them violates the Heisenberg uncertainty principle. But without such classical scene-setting, the quantum calculations are quite impossible." (Chang, 2015.p. 198

Rejecting the theory-driven point of view

Incompatible

Quantum formalism with Heisenberg's principle

✗

Classical theory: BOA introduces a classical particle

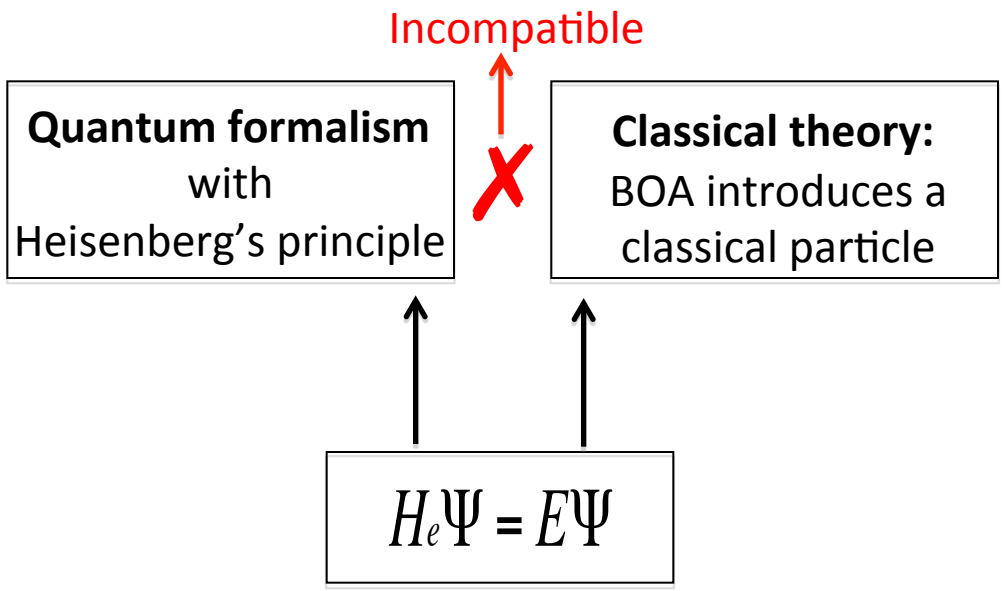
$$H_e\Psi = E\Psi$$

- Due to the theoretical incompatibility we cannot think of this model as a process of de-idealization of the theory

↓

The quantum quemists "may draw concepts out of context, and re-use the concept in a manner not admissible to the theory in which the concept was first introduced" (Hettema 2012, p. 337)

Rejecting the theory-driven point of view



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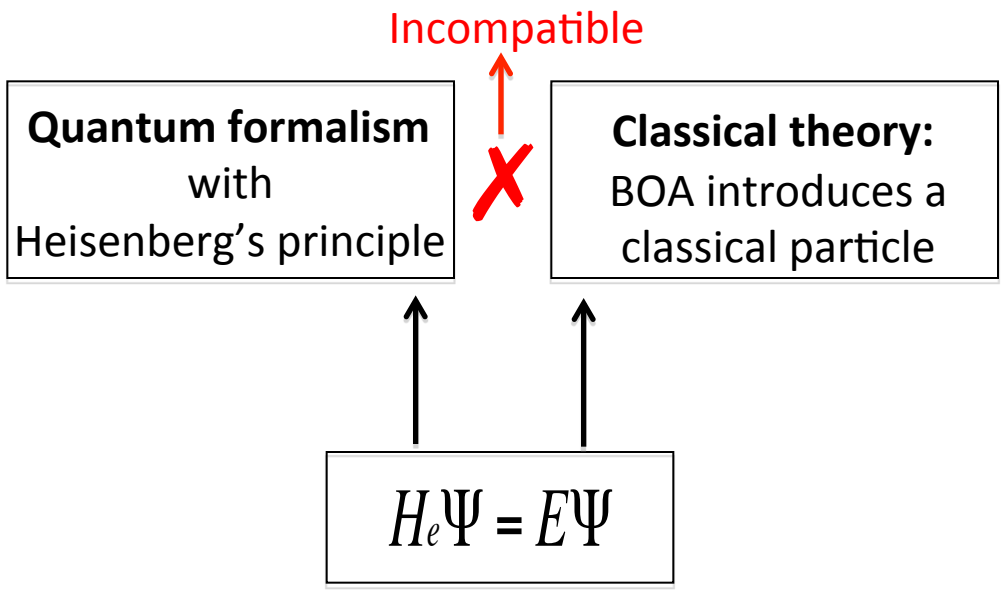
- Models in quantum chemistry do not depend on theories

↓

Models are autonomous and take from theories what they need

Rejecting the theory-driven point of view



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The quantum quemists "may draw concepts out of context, and re-use the concept in a manner not admissible to the theory in which the concept was first introduced" (Hettema 2012, p. 337)

- Models are not truth-makers
- Models in quantum chemistry do not depend on theories

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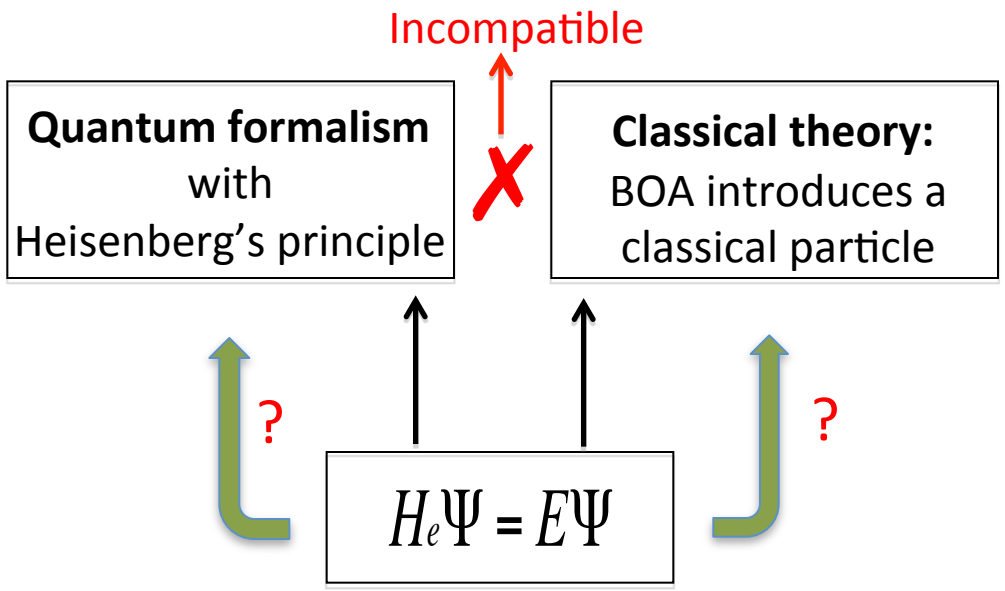
Models are autonomous and take from theories what they need

Rejecting the theory-driven point of view



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The quantum quemists "may draw concepts out of context, and re-use the concept in a manner not admissible to the theory in which the concept was first introduced" (Hettema 2012, p. 337)

- Models are not truth-makers

↓

When a model involves two incompatible theories, which one is confirmed?

- Models in quantum chemistry do not depend on theories

↓

Models are autonomous and take from theories what they need

Conclusions

- The fact that theories are necessary does not imply a dependence of models from theories.

- In quantum chemistry theories have an instrumental role. They are useful, among many other things, to build a successful model. That´s why the models are not their truth-makers

- The molecular models are autonomous: they take only what they need to explain the phenomenon without taking into account whether theories involved are incompatible or contradictory. That means that theories do not include the set of their models because a model is not model of a theory.

- This independencies are not relative or historical, rather they belong to the core of the quantum chemistry

↓

"So one might say that Schrödinger's quantum mechanics, **right from its very first use for a real-life system, was born with the nucleus-clamping assumption**. It should be stressed again that this is not something that arises from the need for approximation, but something woven into the very fabric of elementary quantum theory" (Chang 2015, p 199)

¡MUCHAS GRACIAS!