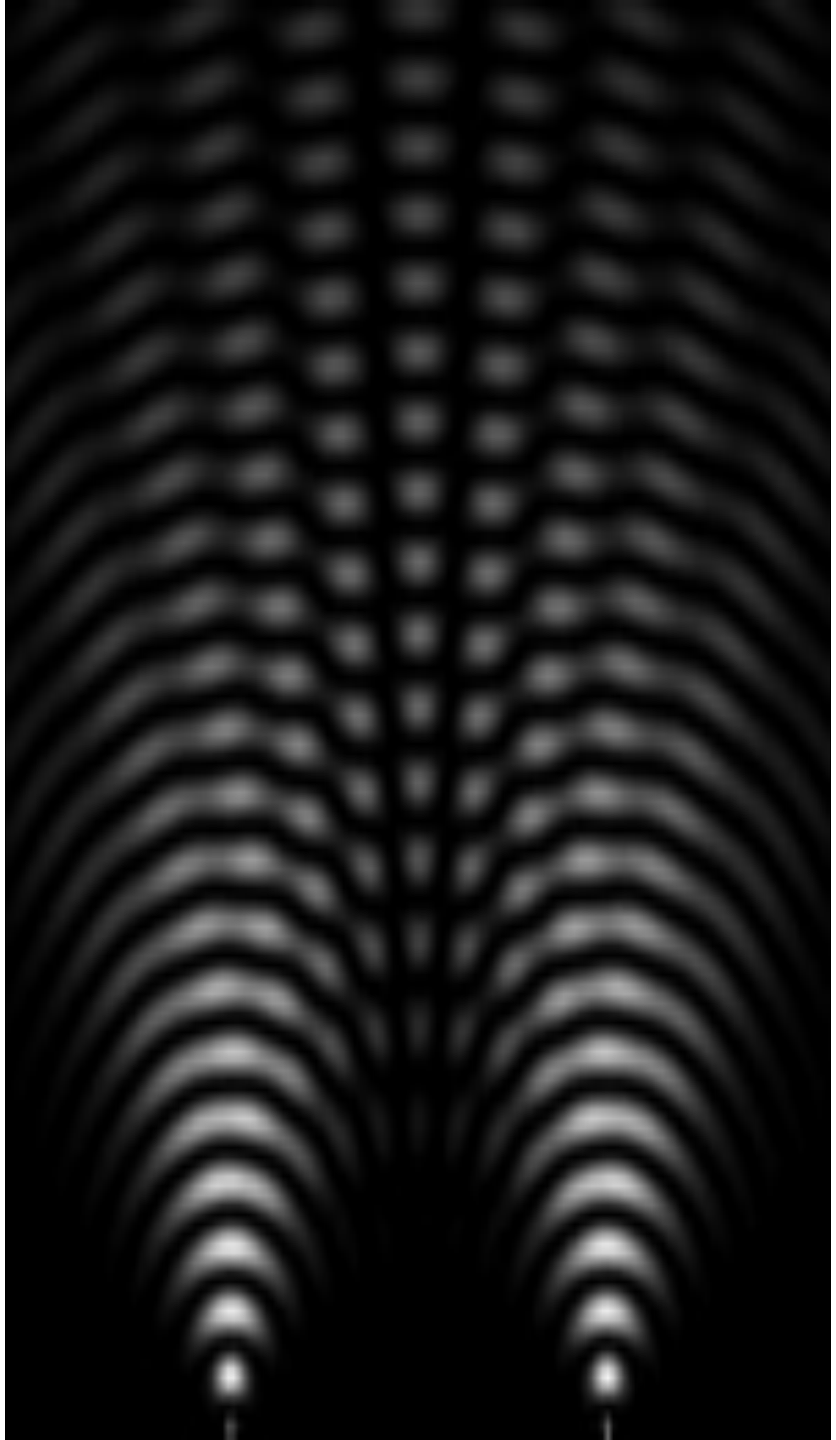

The chemistry between Newton and Schrodinger

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"Those who educate children well are more to be honored than they who produce them; for these only gave them life, those the art of living well."

- Aristotle (384-322 BCE)

"To me there has never been a higher source of earthly honor or distinction than that connected with advances in science."

– Sir Isaac Newton (1642-1727)

Outline

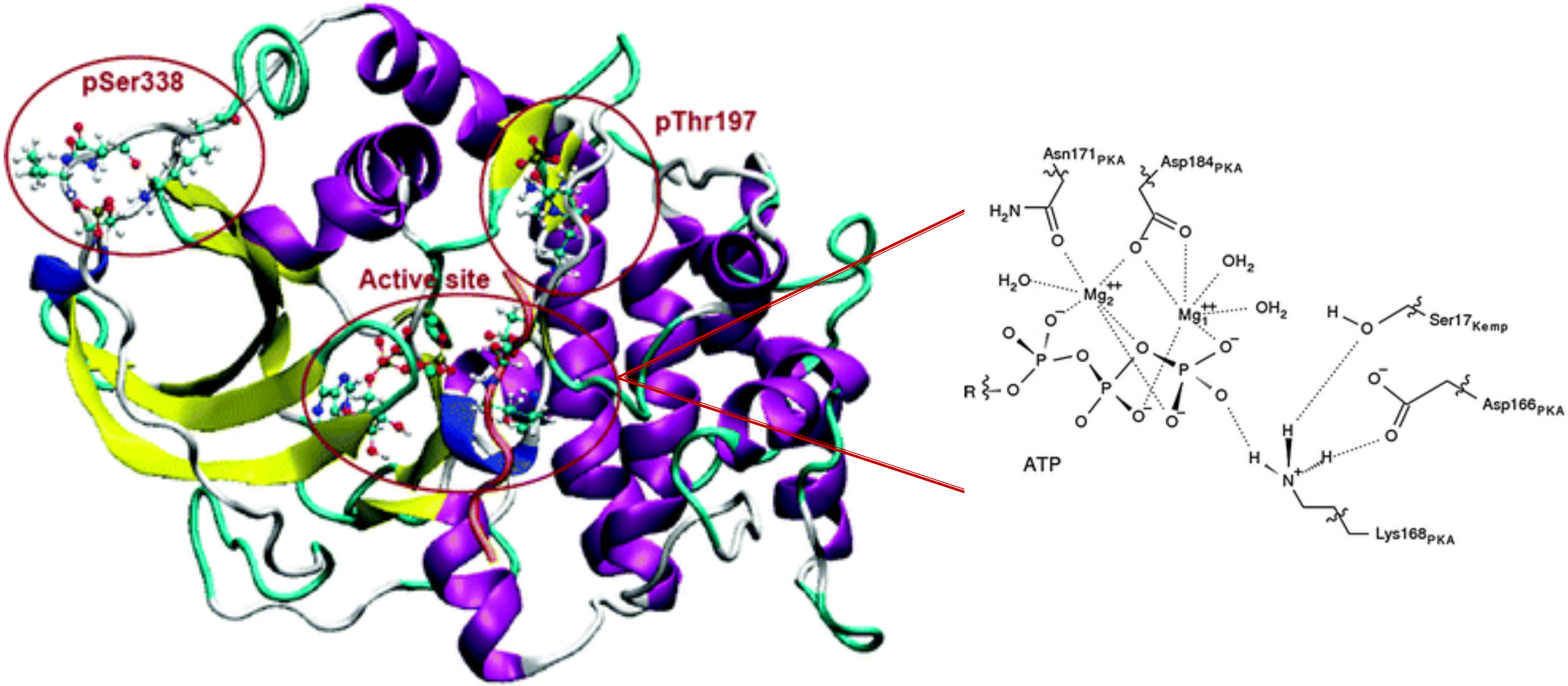
- Why are we talking about this?
  - Understanding the world around us
  - Nobel Prize!
- The classical world through two slits
  - Particles: Newton, Lagrange and Hamilton
  - Waves: Huygens, Young
- It’s 1926 and the world gets stranger: quantum mechanics
  - Bohr, Einstein, Schrodinger, Heisenberg, Born, Dirac, and Feynman
- Chemistry: a foot in two worlds

The Nobel Prize in Chemistry 2013

"for the development of multiscale models for complex chemical systems"

"…they managed to make Newton's classical physics work side-by-side with the fundamentally different quantum physics."

QM/MM study of protein kinase



Protein Kinase facilitates transfer of a phosphate (PO_4^-) group:
relevant to many auto-immune disorders

Newton and Schrödinger’s cat

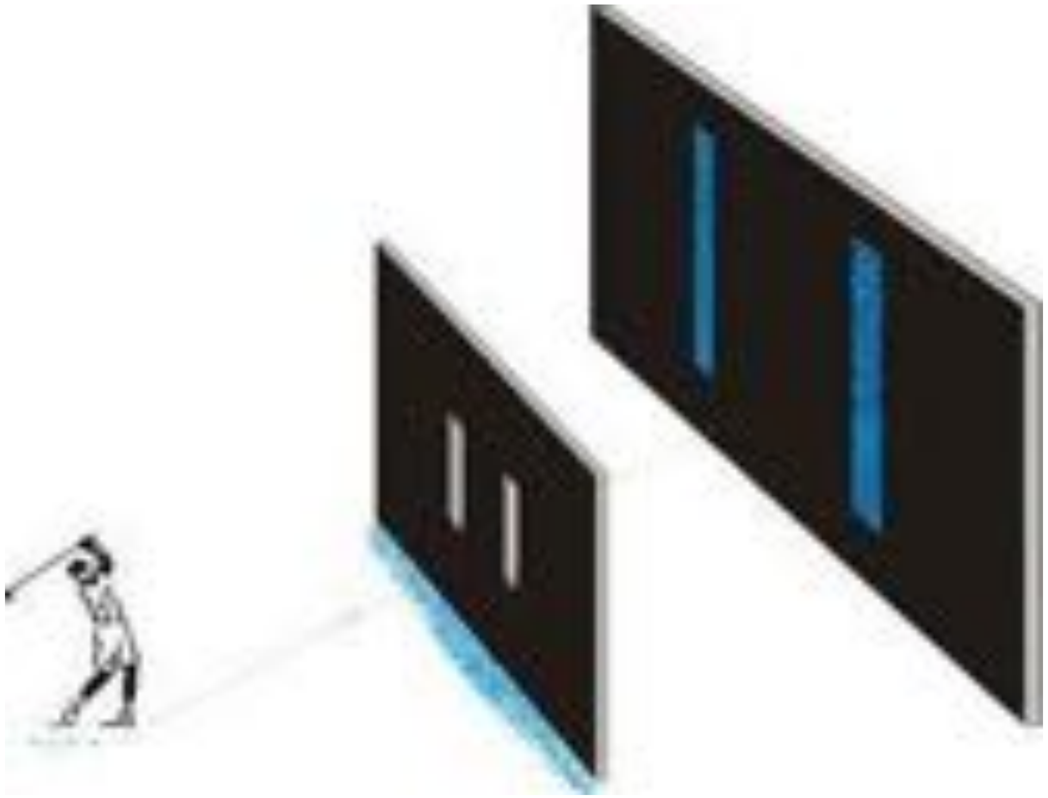
The methods of scientific research

- Unify: seek the underlying physics that unites disparate theories

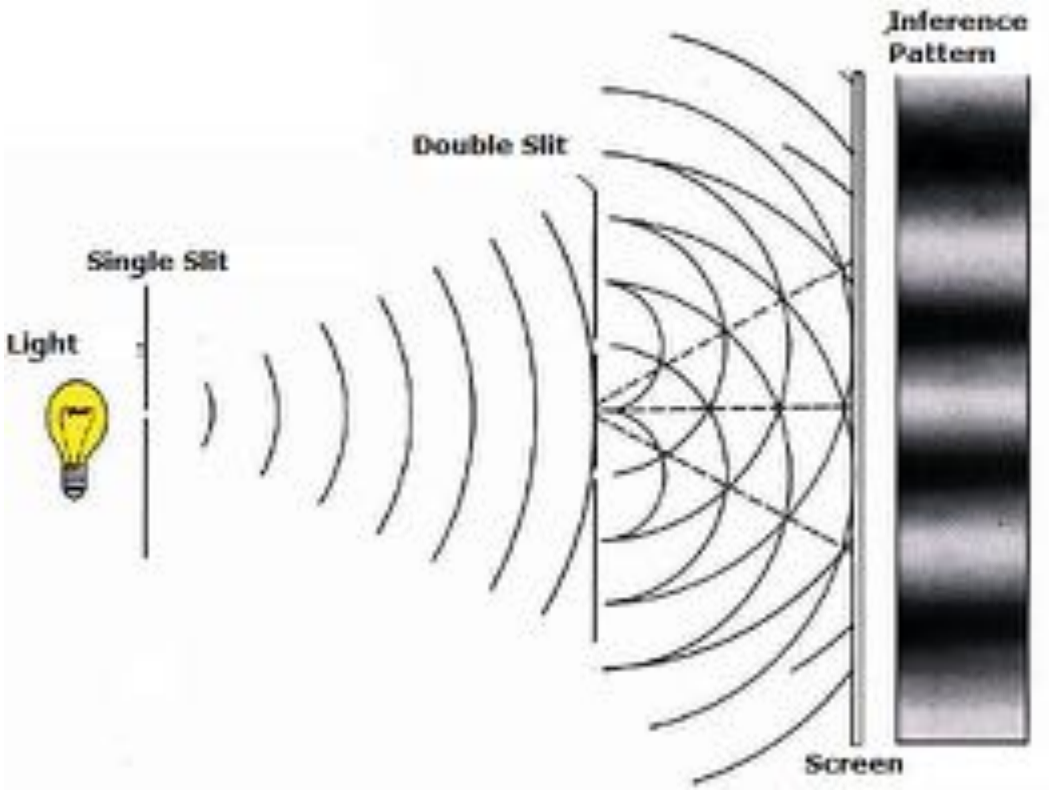
- Reformulate: understand an existing theory in a different way

- Discover limits: identify new phenomena transcending current theories

Classical double slit experiment



Classical Particles



Classical Waves

Thomas Young, 1803: set out to disprove Newton's corpuscular theory in favor of Huygen's wave theory of light.

Things start to be 'quantum'

- Boltzmann (1877): energy levels of molecules may be discrete
- Heinrich Hertz and Einstein (1887): photoelectric effect
- Max Planck (1900): black-body radiation
- Neils Bohr (1913): on the constitution of atoms and molecules
- Louis Debroglie (1924): wave-particle duality
- 1926: Heisenberg develops matrix mechanics
  Schrödinger publishes wave equation

Life after 1926

- 1927: Heisenberg uncertainty principle
  Dirac brings together QM and Einstein's special relativity
  Heitler and London pioneer quantum chemistry

- 1927-1940: Dirac, Pauli, Feynman – Quantum Field Theory

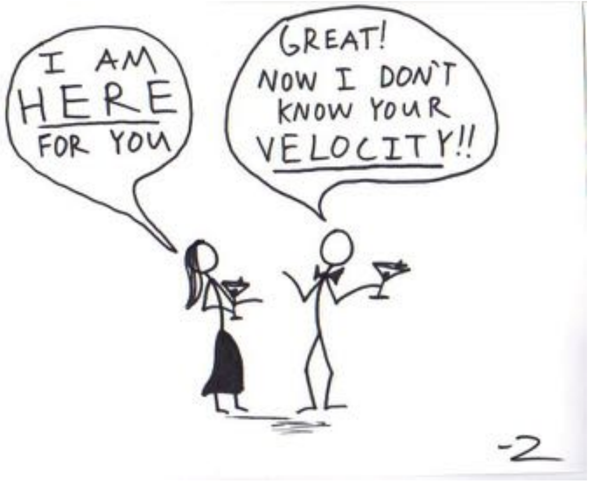
- 1975: Politzer, Gross and Wilczek – Quantum Chromodynamics

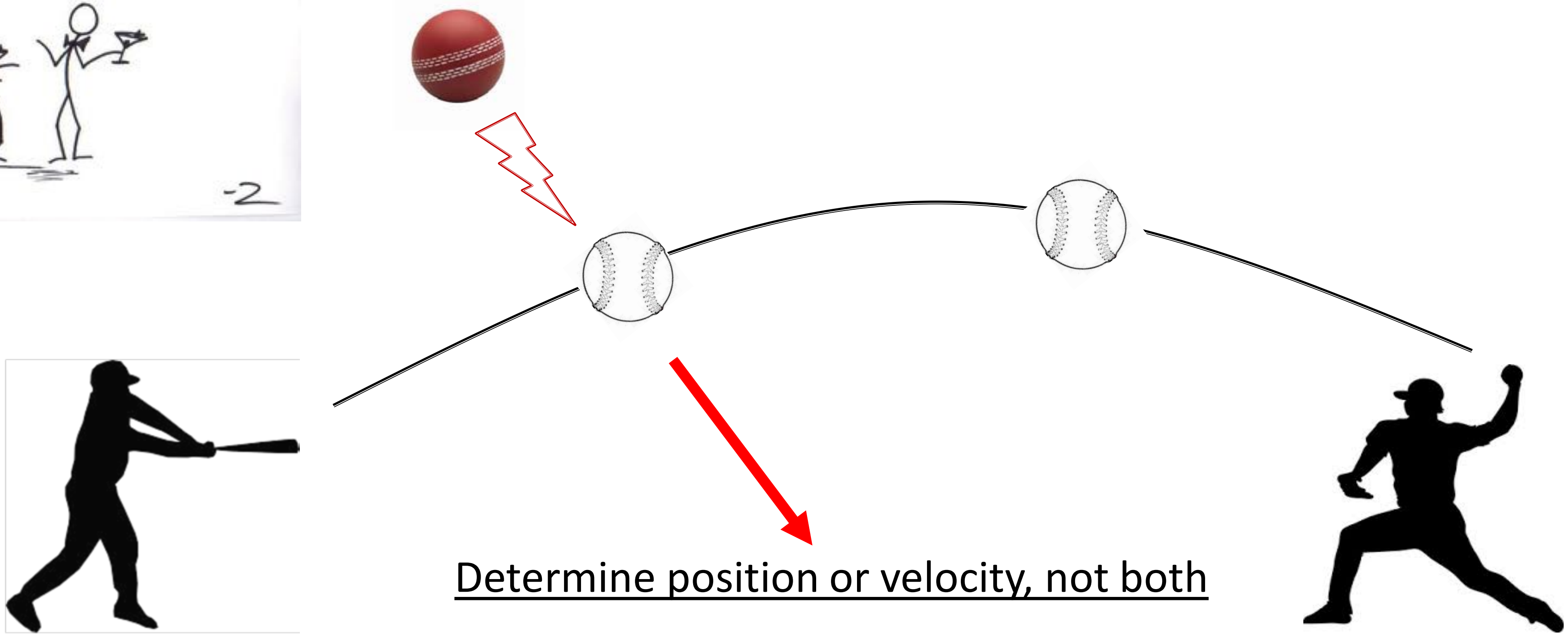
- 1979: Weinberg, Salam and Glashow – unified electroweak forces

- 2013: Confirmation of Standard model – theory of almost everything

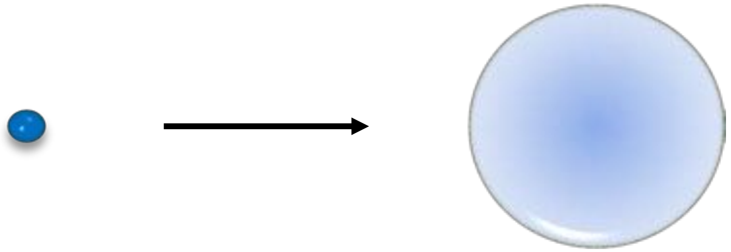
Uncertainty principle

Consequence of Wave-Particle Duality!



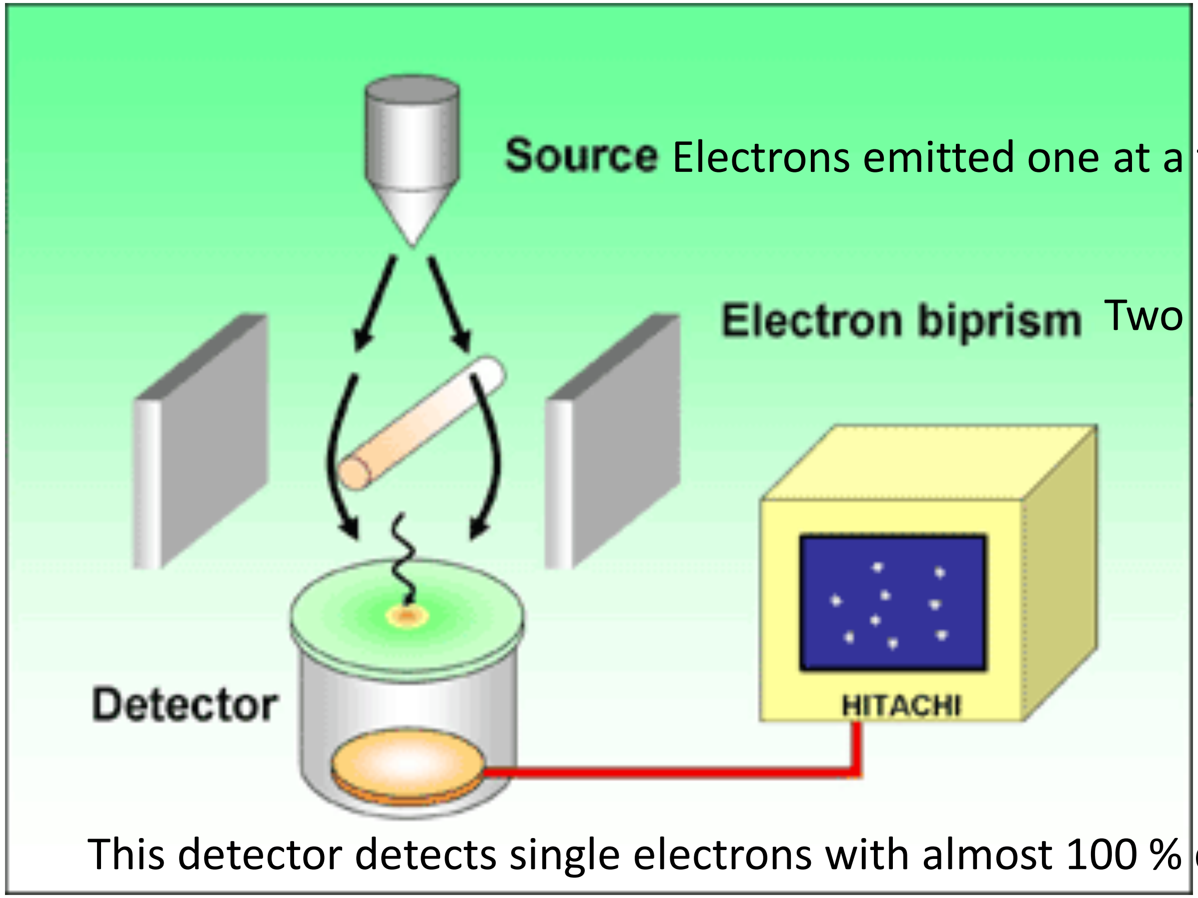


Determine position or velocity, not both



I, at any rate, am convinced that *He* does not throw dice - Einstein

Performing the quantum double-slit experiment



Electrons emitted one at a time from source

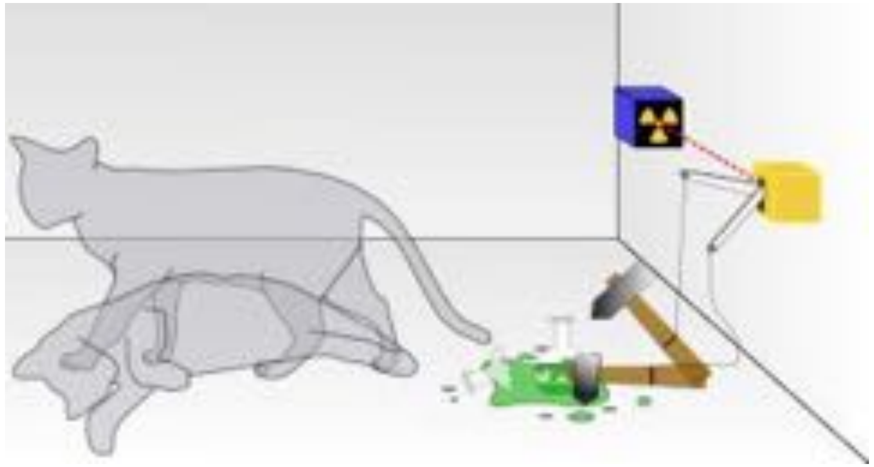
Two parallel plates and a fine filament between them

This detector detects single electrons with almost 100 % detection efficiency.

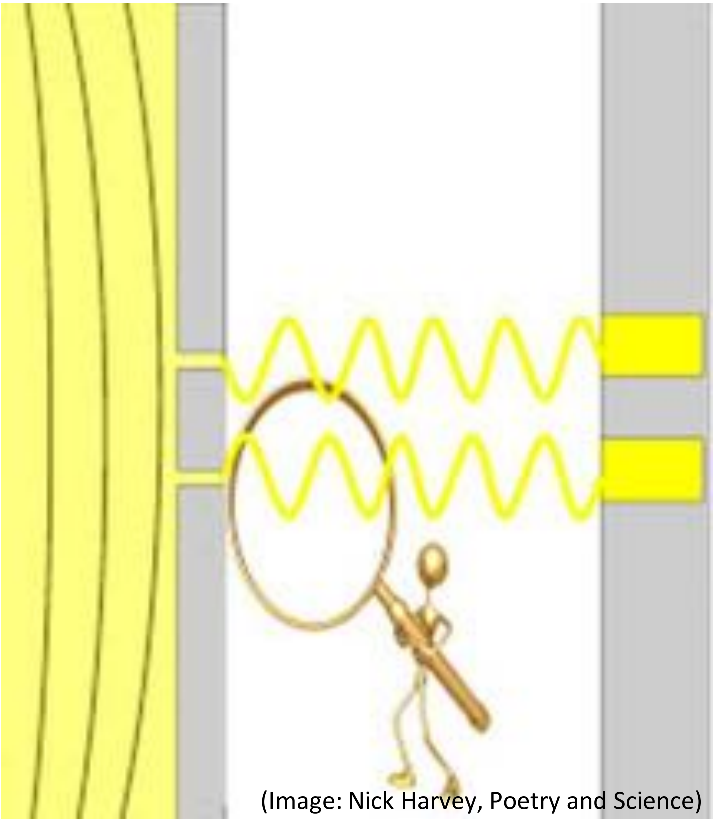
Electron double-slit experiment

The observer paradox

Copenhagen Interpretation of a measurement:

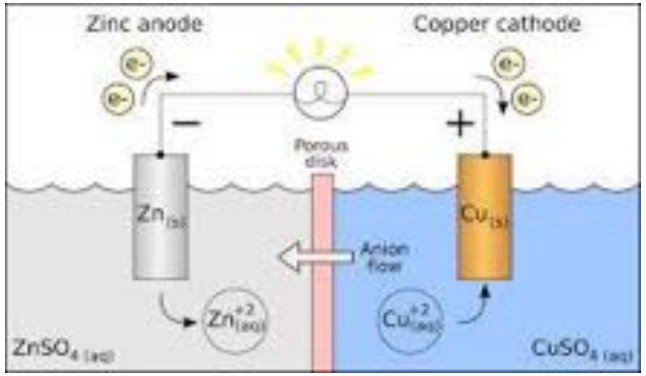


Schrödinger's cat: reduction ad absurdum

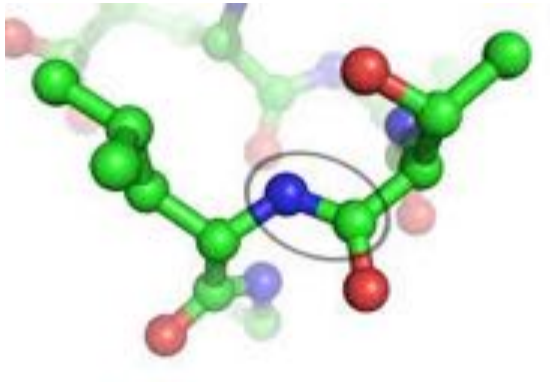


(Image: Nick Harvey, Poetry and Science)

The act of 'observation' interacts with the quantum system



Connection to Chemistry?



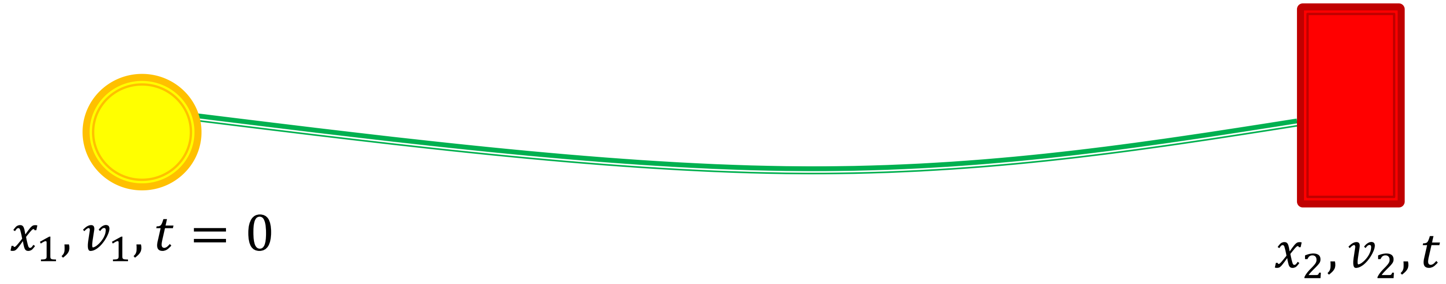
- Chemical reactions involve breaking, making, and changing bonds
- Changing bonds involves moving electrons and atoms: quantum mechanics.
- For bonds not explicitly involved in chemical reaction: classical mechanics.

What is a clever way to combine the two in one <u>uniform</u> framework?

Classical mechanics

- Deterministic paths
  - Initial position
  - Initial velocity
  - Forces

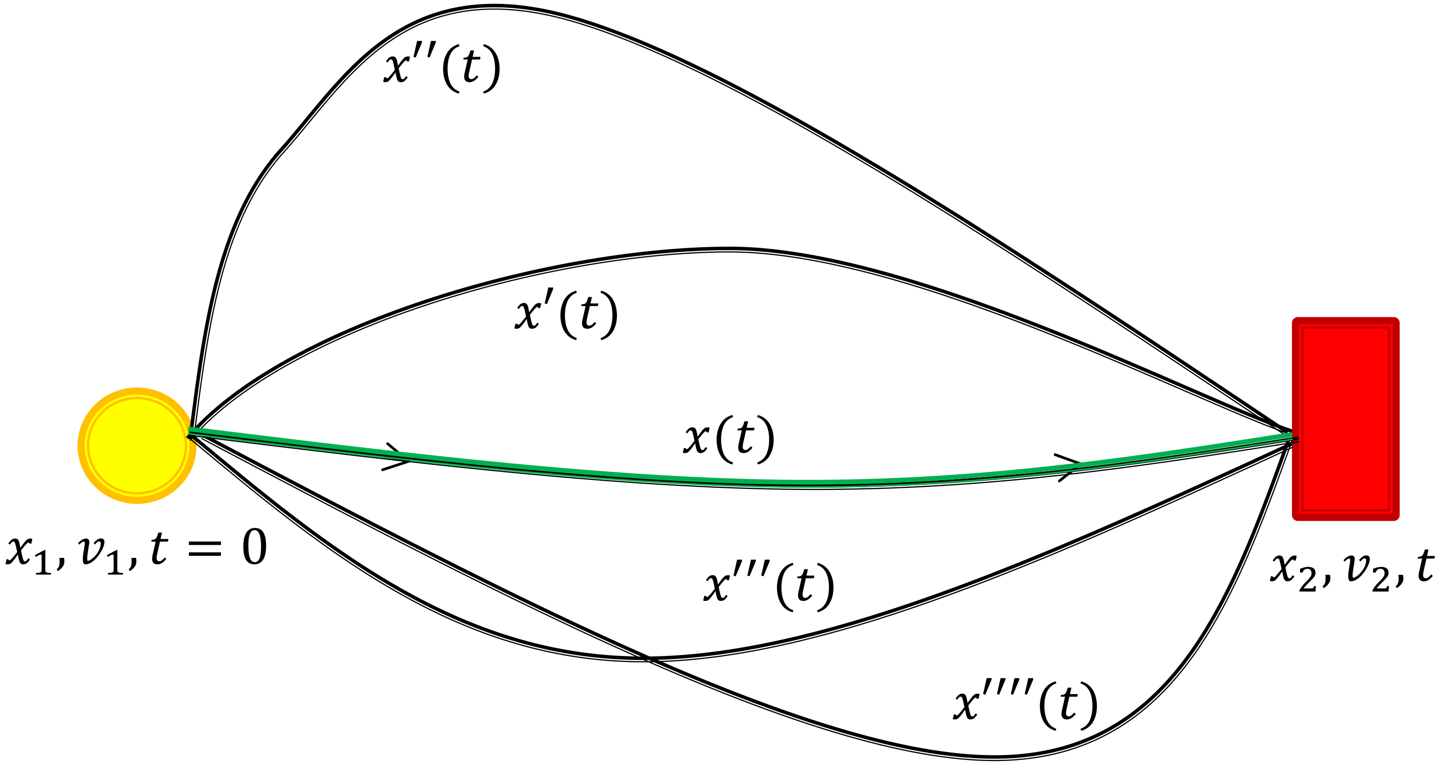
- Newton's second law: $F = ma$



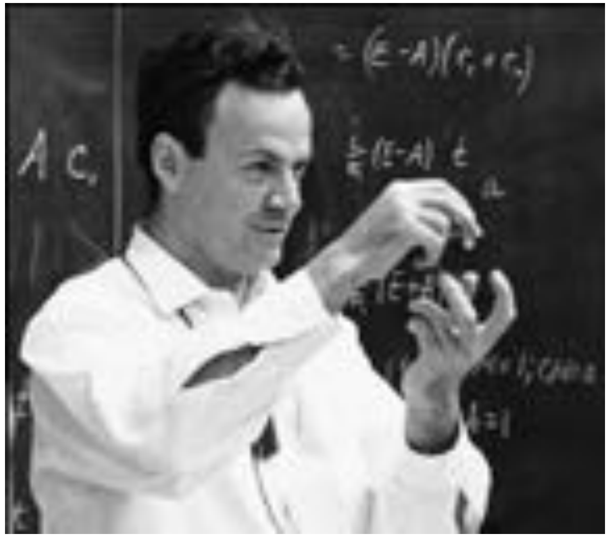
Reformulate: Lagrange and Hamiltonian

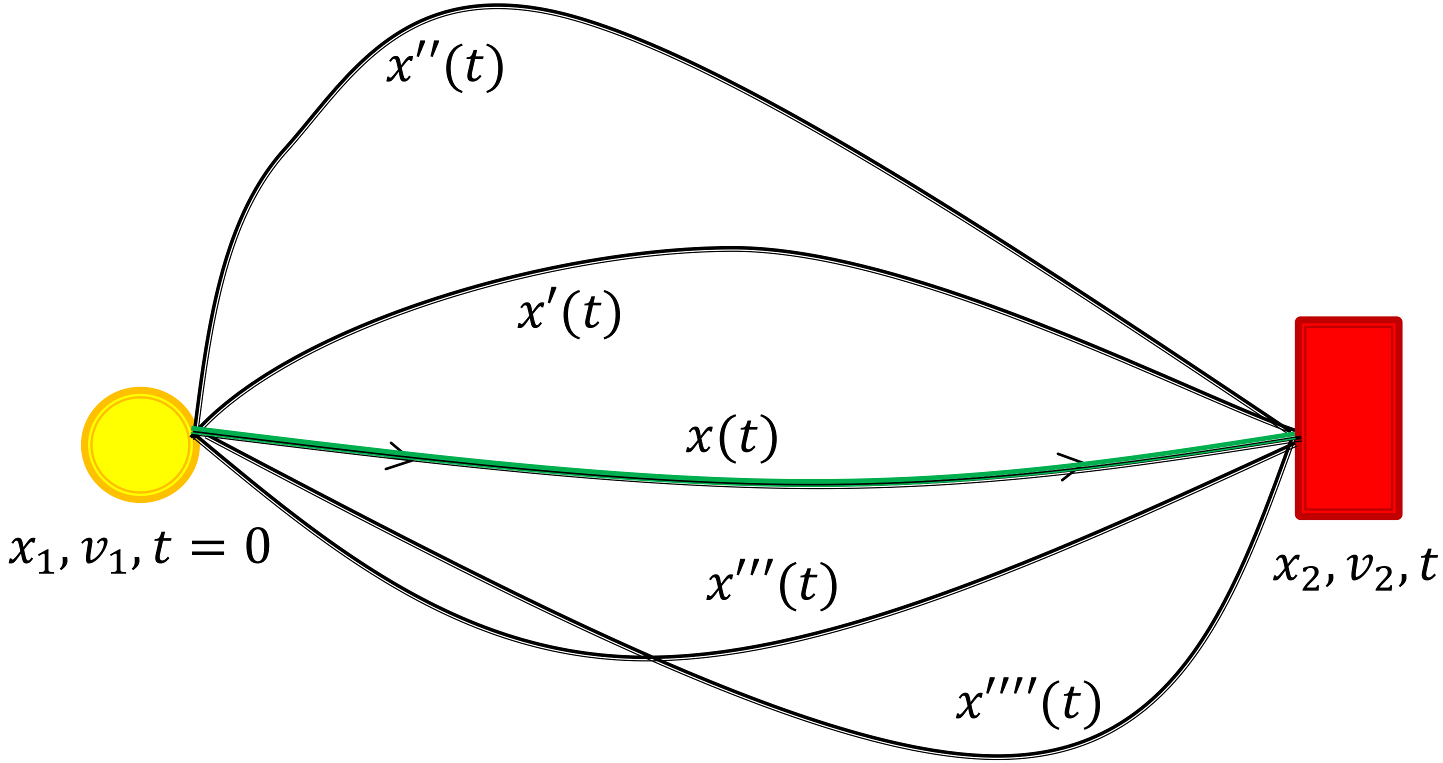
- Lagrange introduce action: associate $S[x(t)]$ with classical path $x(t)$

- Hamilton’s principal of least action: $\delta S = 0$



Unify ideas: Feynman Path Integral

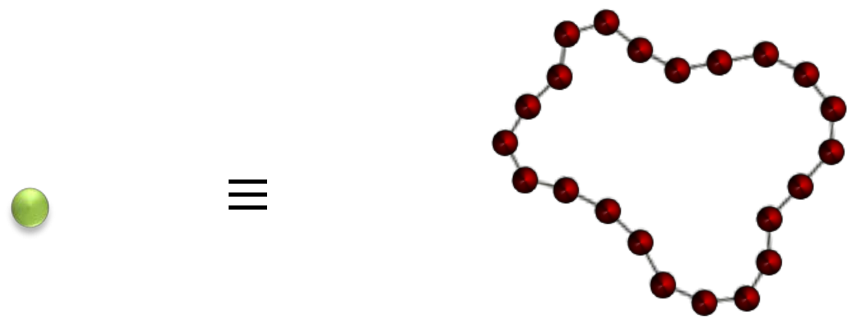




$$\mathrm{P}\big((x_1, v_1, t = 0) \rightarrow (x_2, v_2, t)\big) \propto \sum_{paths} e^{\frac{iS[x_{path}(t)]}{\hbar}}$$

Path-Integral representation of quantum mechanics

- A quantum particle behaves like a collection of classical particles



- A quantum particle that behaves like 1 classical particle is a classical particle

- The number of classical particles that describe a quantum particle depends on temperature and/or energy

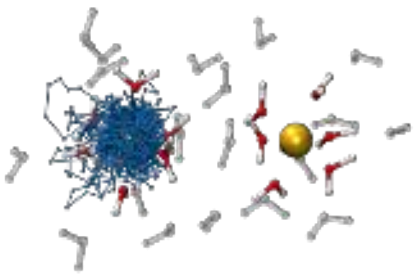
Dynamics of electron in water

Solvated electron problem: important for all charged particle moving through solvent.

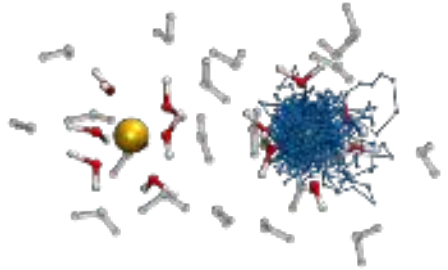
Applications: Battery and electrode design, charge transfer in condensed-phase reactions and many more.

(Menzeleev et al, J. Chem. Phys. , 2009)

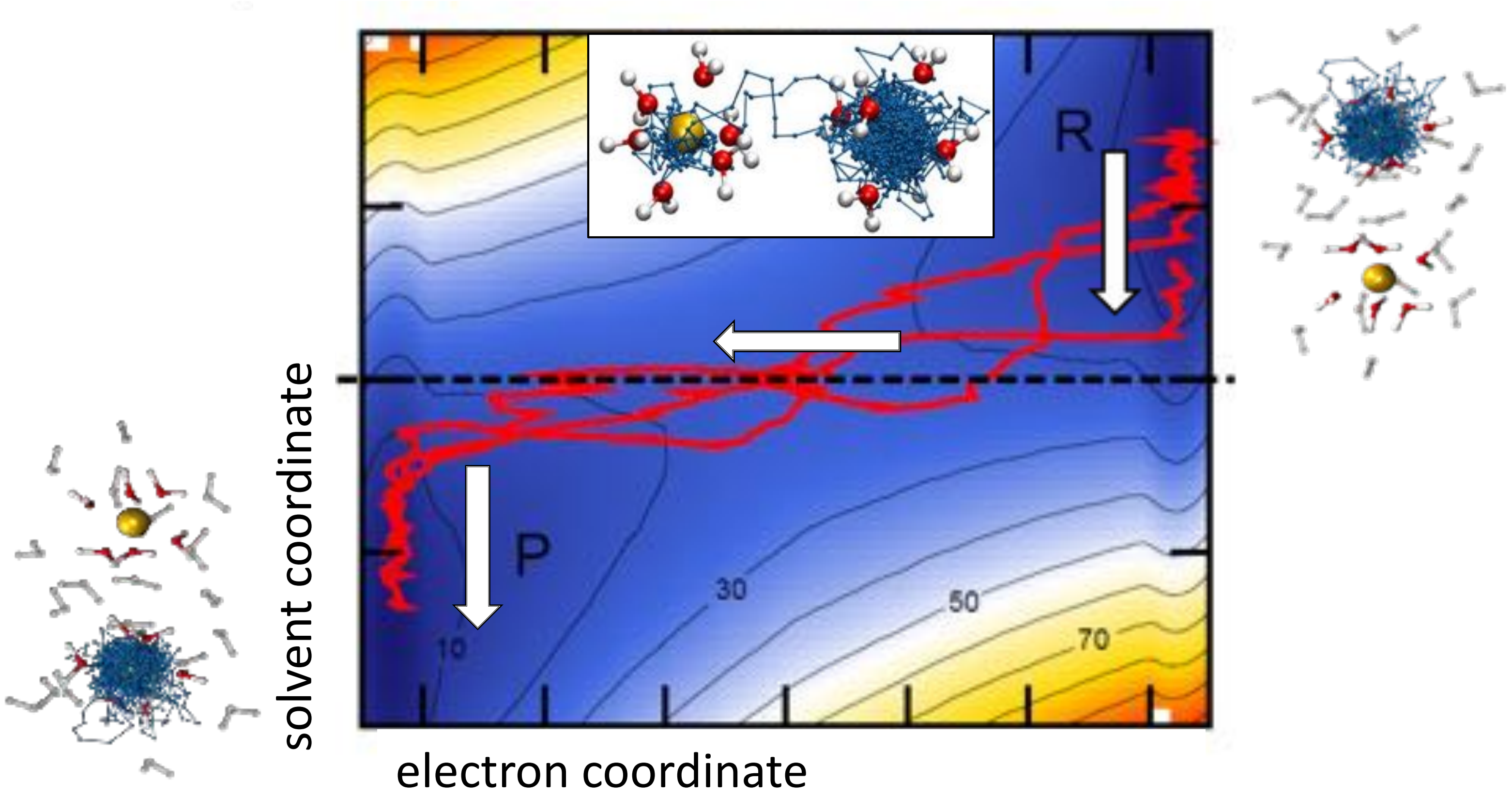
Electron transfer in solution



$$Fe^{2+} + Fe^{3+} \rightarrow Fe^{3+} + Fe^{2+}$$



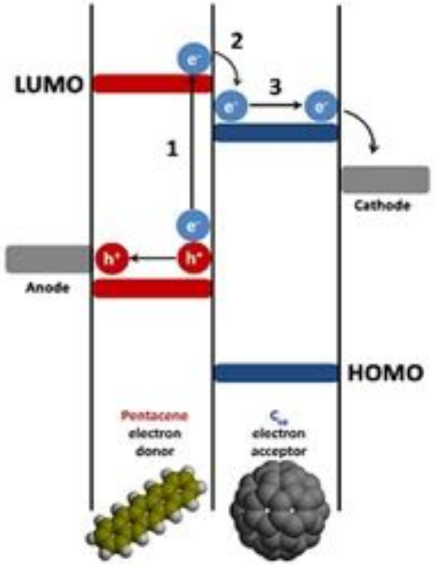
System size: 430 water molecules, 2 metal ions, 1024 path-integral ‘beads’ for electron.



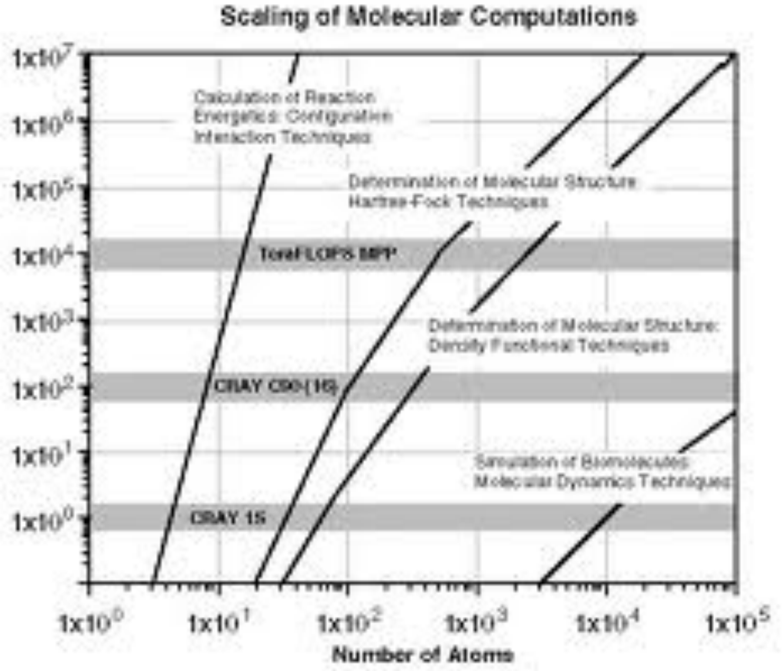
(Menzeleev et al, J. Chem. Phys. , 2010)

Current research in theoretical chemistry

- Understanding structure-function relations in Biological systems



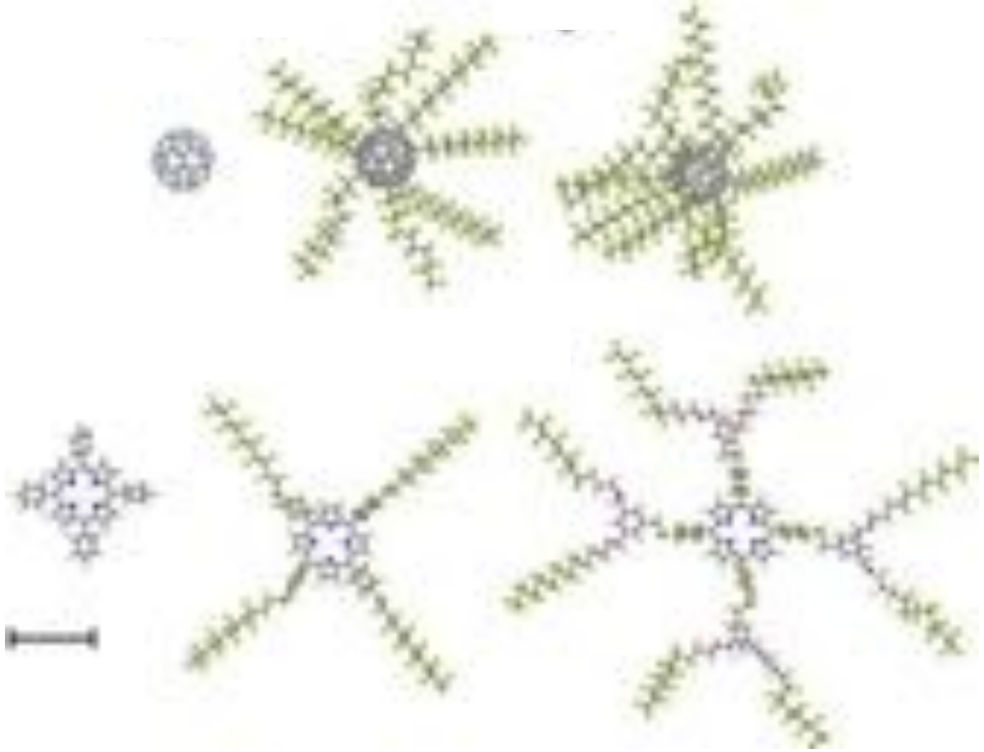
- Designing efficient renewable energy materials

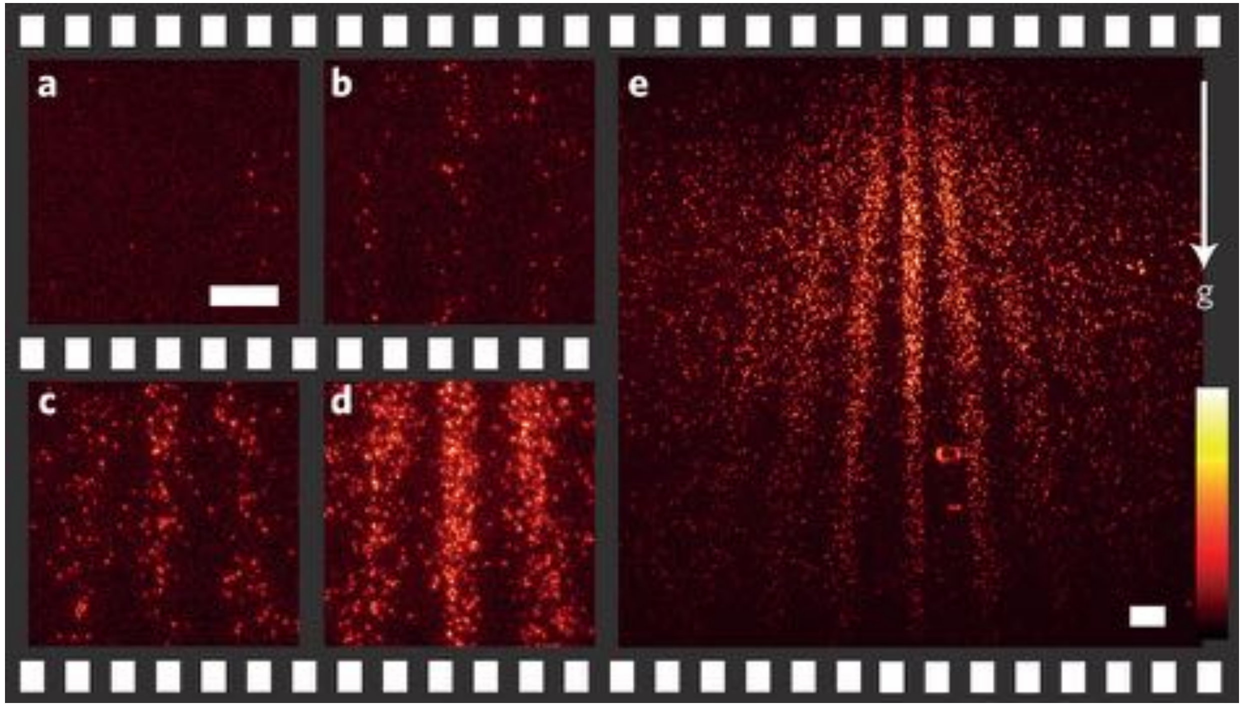


- Computational complexity challenges

Frontiers in quantum mechanics

How big is ‘classical’?

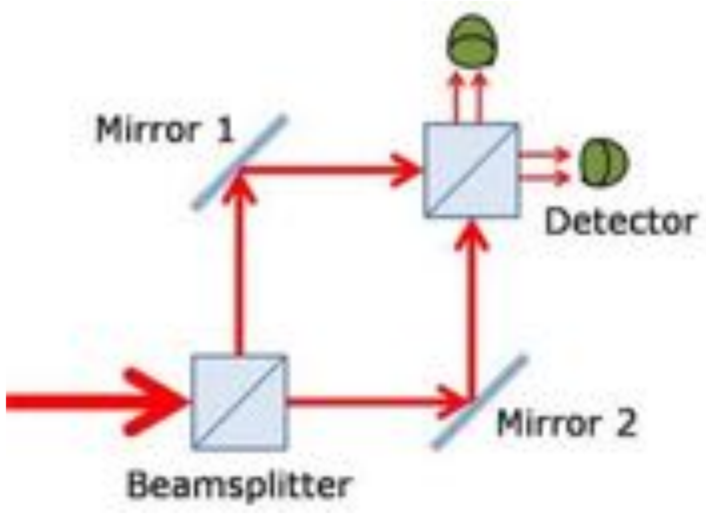




S. Gerlich et al, “Quantum interference of large organic molecules”, Nature 2, 263 (2011).
T. Juffmann et al, “Real-time single molecule imaging of quantum interference”, Nature Nanotechnology, 7, 297 (2012).

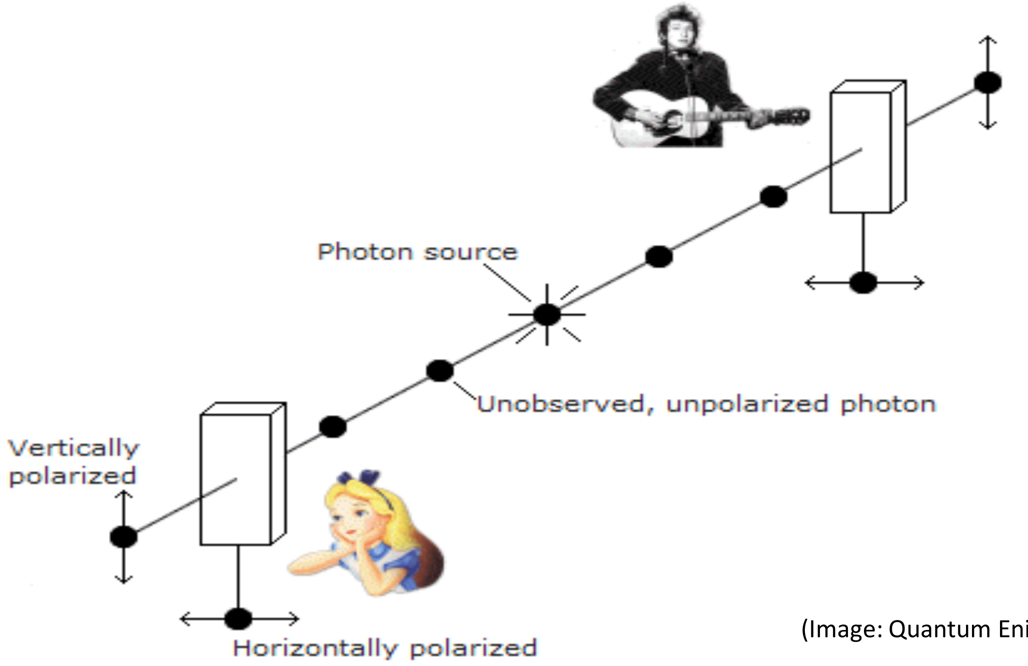
Frontiers in quantum mechanics

Role of observer: double-slit experiment



V. Jacques et al, "Experimental Realization of Wheeler's Delayed-Choice Gedanken Experiment", Science 315, 966 (2007).

Einstein-Podolsky-Rosen (EPR)



(Image: Quantum Enigma)

Quantum mechanical origin of gravity

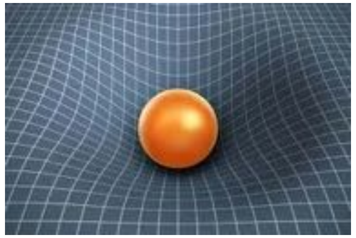


Image: koya/shutterstock

‘Therefore, just as the doctor is said to heal a patient through the activity of nature, so a man is said to cause knowledge in another through the activity of the learner’s own natural reason and this is teaching’

- Thomas Aquinas (1225-1274)

THANK YOU!