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## Strong Influence of Molecular Interactions over Large Distances and Its Consequences

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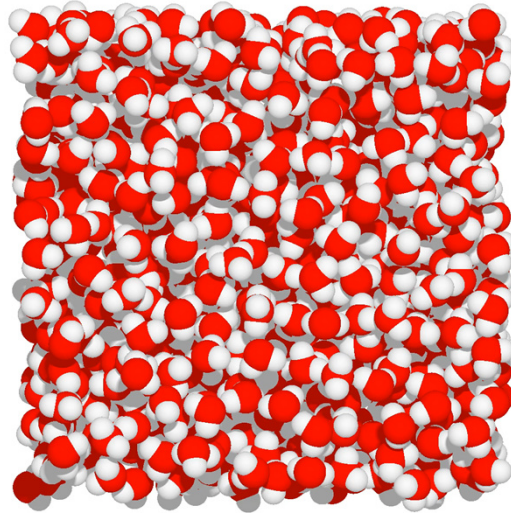


### questions to be answered

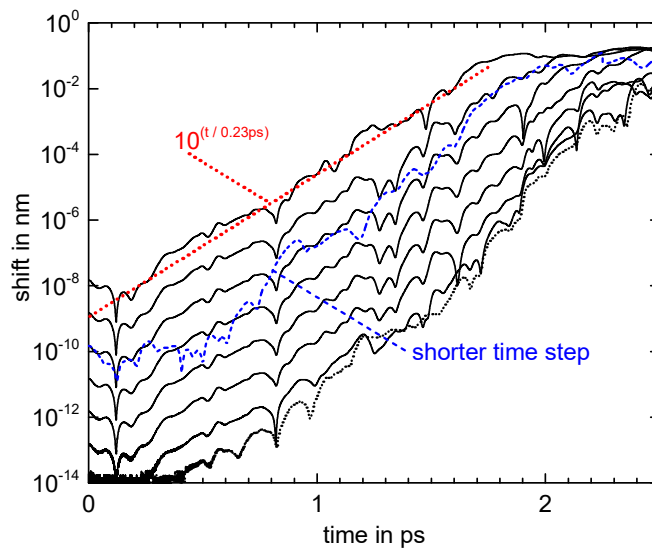
- How do small perturbations influence molecular motion?
- How do molecules interact over large distances?
- What are the consequences for our world view?



## liquid water, 37°C, periodic boundaries



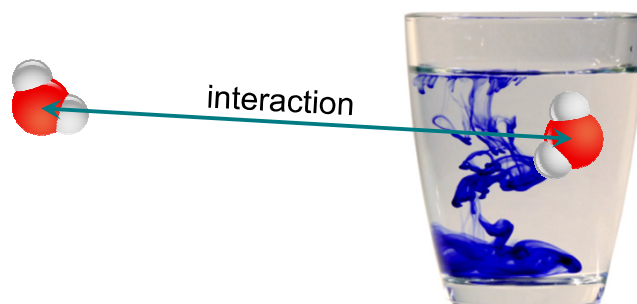
## Lyapunov instability in liquid water at 37°C



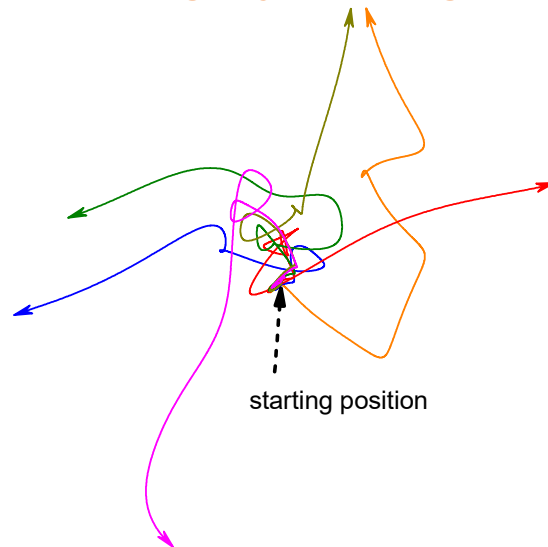
## consequences

- deterministic chaos, Lyapunov time
- prediction every 0.23 ps further into the future requires one more decimal digit in start coordinates and calculations, e.g. 33 ps  $\Rightarrow$  144 digits
- thus: cannot be predicted over intermediate times
- this is statement only about prediction, not about reality itself

## thought experiment

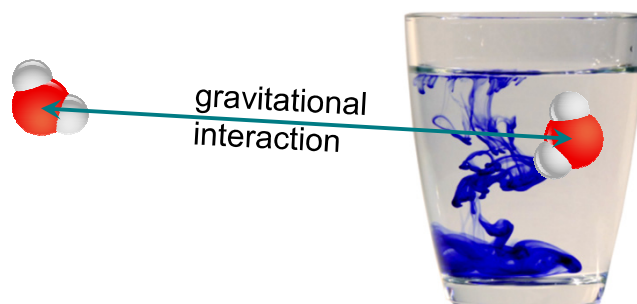


## randomization after slightly differing initial perturbations

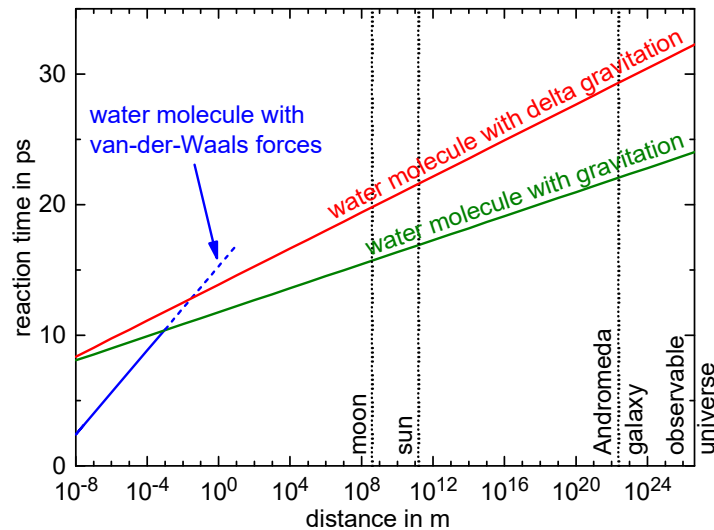


## question:

- How long does it take until the interaction leads to an observable bifurcation?
- bifurcation = shift by molecular diameter



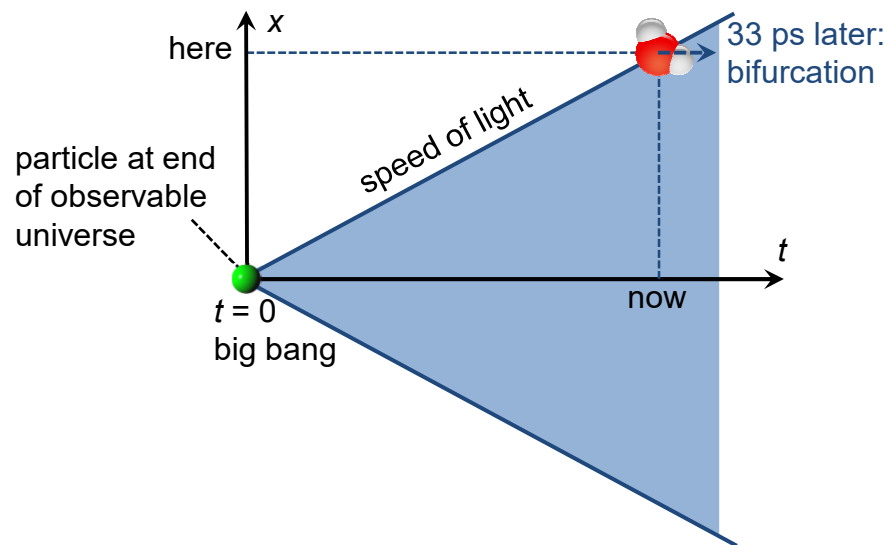
## influence between two water molecules



## picture

- all particles send information
- travels with speed of light
- any particle experiences at every moment the sum of all interactions with all particles
- interactions superimpose linearly
- reacts to this interaction
- if any faraway particle would have been in a slightly different place, after at most 33 ps the observed particle would react differently at any multi-furcation

## cone of interaction



## consequences

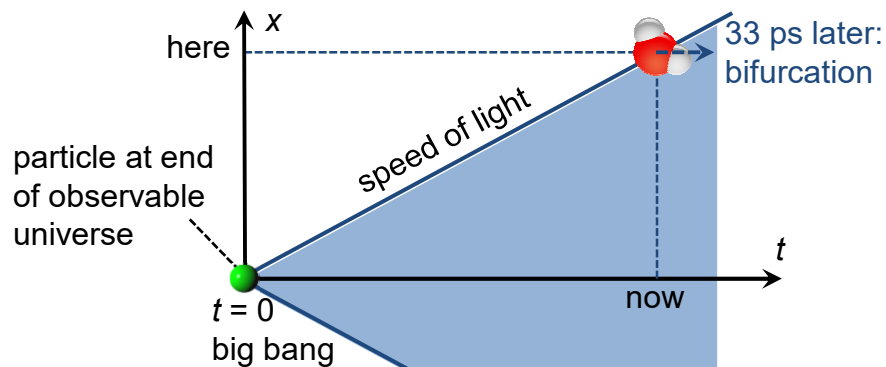
- all particles influence each other within 0 to 33 ps on universal scale (possibly much faster)
- but: speed of light
- this is about **interaction in reality**, not only about prediction
- randomizing effect
- even in a fully deterministic world view

## reversal of time in physical laws (our description of reality)

- e.g. conservation of energy and momentum
- Newtons laws of motion
- but entropy reduction improbable:



## cone of interaction

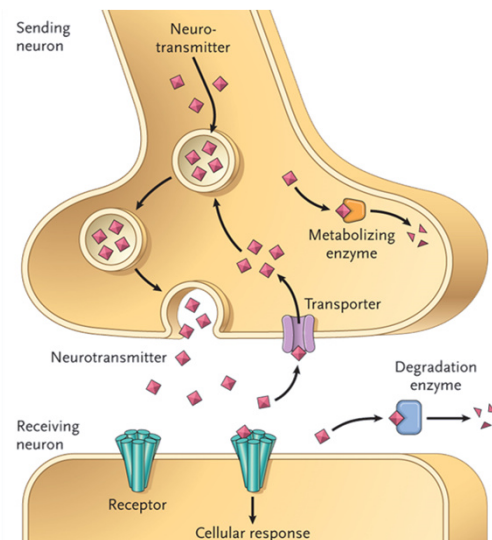


## conclusions

- physical laws may be time reversible
- initial conditions can freely be chosen only in forward direction of time
- in backward direction: vast multitude of conditions, in effect: reversal only possible starting from system that developed in forward direction

## free-will decisions?

- decision = bifurcation
- synapse:
  - area  $0.04 \mu\text{m}^2$
  - distance to neuron 20 nm
  - concentration 10 to 25  $\mu\text{mol/l Ca}^{2+}$
- 7 to 20 ions  $\text{Ca}^{2+}$  make a difference
- molecular level involved
- free-will decision will have random aspects
- we are not able to predict the decision, i.e. have to regard it as free





## conclusions

- interactions over arbitrary distances lead to molecular reactions after at most 33ps
- deterministic chaos is not only about predicting reality but about interactions in reality leading to true unpredictability
- direction of time in physical laws: determined by initial conditions
- free will: randomness even in fully deterministic system
- quantum physics: randomness even if deterministic?
- Pfennig, A. (2018): On the strong influence of molecular interactions over large distances. European Physical Journal D - Atoms, Molecules, Clusters & Optical Physics, 72 (March, paper 45), 1-8.

## Ernst Mach

There is no cause nor effect in nature;  
nature has but an individual existence;  
nature simply is.

Ernst Mach: The Science of Mechanics.  
A Critical and Historical Account of its Development.  
Translated by Thomas J. McCormack.  
The Open Court Publishing Co., Chicago, 1919.

in other words:

Reality does not care about our futile attempts to describe it.

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backup slides



## interaction of distant particle 1 for $\Delta t_{interaction}$

$$F = G \frac{m_1 m_2}{r_{1,2}^2}$$

$$F = m_2 a$$

$$a = \frac{\partial^2 s}{\partial t^2}$$

$$\Delta t_{interaction} \Rightarrow \Delta s_0$$

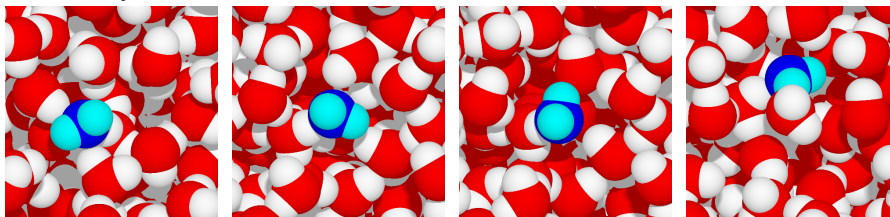
$$\Delta s = \Delta s_0 10^{t/t_{scale}}$$

$$\Delta t_{reaction} = t_{scale} \left( \log_{10} \frac{2\Delta s}{Gm_1} + 2 \log_{10} r_{1,2} - 2 \log_{10} \Delta t_{interaction} \right)$$

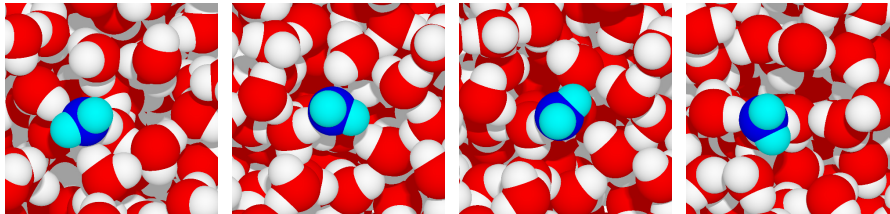
- $m_1$  – mass of distant particle
- $m_2$  – mass of observed particle
- $r_{1,2}$  – distance between particles
- $F$  – force acting between particles
- $t$  – time
- $\Delta s_0$  – initial shift of observed particle
- $t_{scale}$  – 0.23 ps

## influence by a faraway water molecule

isolated system



interacting with single water molecule at the end of the observable universe



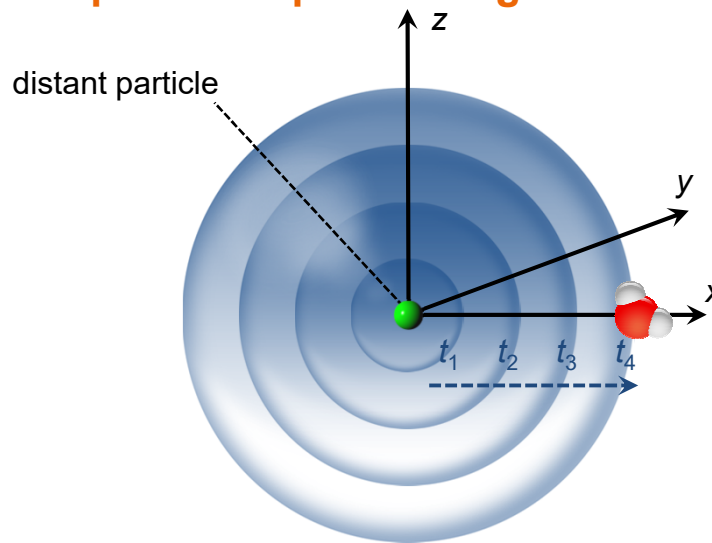
0.0 ps

31.9 ps

32.0 ps

33.0 ps

## interaction spheres at proceeding time



## cone of interaction

