Can Chemistry be Computationally (and not Only Theoretically) Reduced to Quantum Mechanics? Cognizability Explains Dirac's Relation Between Fundamental Physical Constants

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1. Can Chemistry be Reduced to Quantum Physics? The Original Question

- *Fact:* Schrödinger equation describes the dynamics of an arbitrary system of elementary particles.
- *Comment:* we need relativistic (Dirac's) equations.
- *Conclusion:* all the chemical properties should follow from the Schrodinger equation.
- *Historical fact:* in the 1920s, some over-optimistic physicists predicted the end of chemistry.
- *Future (?):* chemistry will be reduced to quantum physics.
- *Historical fact:* chemistry did not end.
- *Explanation:* from the the computational viewpoint, this reduction was only possible for the simplest atoms.

2. Can Chemistry be Reduced to Quantum Physics? Current Optimism

- *General progress:* computers have become extremely fast.
- *Computational chemistry:* many chemical properties are computed based on quantum physics.
- *Reasonable assumption:* in principle, chemical phenomena are cognizable.
- *Future (?):* in principle, all chemical properties can be *computationally* derived from the quantum equations.
- *Caution:*
  - this assumption is not about the ability of the *existing* computers;
  - it is about *potential* future computers, in which the time of each computational step is small.

3. What We Plan to Discuss in This Talk

- *Fact:* the computation time needed to solve the Schrodinger equation grows with the number of particles.
- *Fact:* the computation time cannot exceed the Universe's lifetime.
- *Conclusion:* a restriction on the size of possible atoms.
- *Interesting corollary:* we explain Dirac's empirical relation $1/\alpha \approx \log_2(N)$ between fundamental physical constants:
  - $\alpha = 1/137.095...$ is the fine-structure constant;
    - $1/\alpha \approx$ size of the largest possible atom;
  - $N \stackrel{\text{def}}{=} T/\Delta t \approx 10^{40}$, where:
    - T is the Universe's lifetime, and
    - Δt is the smallest possible time quantum.

4. Physical Constants: Reminder

- In physics, there are many constants such as the speed of light c, the charge of the electron, etc.
- Most of these constants are *dimensional*: their numerical value depends on the measuring units.
- *Example:* the speed of light c in miles per second is different from km/sec.
- Some physical constants are *dimensionless* (independent of the choice of units).
- *Example:* a ratio between the masses of a neutron and a proton.
- *Fact:* the values of most dimensionless constants can be derived from an appropriate physical theory.
- *Fundamental constants:* cannot be derived.

5. Size of Dimensionless Constants

- *Fact:* the values of most fundamental dimensionless constants are usually close to 1.
- *Application:* we can estimate the values of quadratic terms (with unknown coefficients) and ignore if small:
  - in engineering,
  - in quantum field theory (only consider a few Feynman diagrams),
  - in celestial mechanics.
- *Exceptions:* there are few very large and very small dimensionless constants.
- *First noticed by:* P. A. M. Dirac in 1937.
- Dirac discovered interesting empirical relations between such unusual constants.

6. An Example of a Very Large Fundamental Constant

- *Staring point:* the lifetime T of the Universe ($T \approx 10^{10}$ years).
- *How to transform it into a dimensionless constant:* divide by the smallest possible time interval Δt.
- *fact:* The smallest possible time is the time when we pass
  - through the smallest possible object
  - with the largest possible speed: speed of light c.
- Which of the elementary particles has the smallest size?
  - In Newtonian physics, particles of smaller mass m have smaller sizes,
  - In quantum physics, an elementary particle is a point particle.

7. Dirac's Constant (cont-d)

- *Reminder:* $N = T/\Delta t$, where:
  - T is the Universe's lifetime, and
  - Δt is the time during which light passes through the smallest particle.
- Due to Heisenberg's inequality $\Delta E \cdot \Delta t \geq \hbar$, the accuracy Δt is $\Delta t \approx \hbar/\Delta E$.
- Thus, we are not sure whether the particle is present, so $\Delta E = mc^2$ and $\Delta t \geq \hbar/E = \hbar/(mc^2)$.
- *Conclusion:* the smallest size particle is the one with the largest mass.
- Among independent stable particles – photon, electron, proton, etc. – proton has the largest mass.
- If we divide T by proton's Δt, we get a dimensionless constant $\approx 10^{40}$.

8. Dirac's Relation Between Fundamental Physical Constants

- *Observation:* Dirac noticed that this constant $\approx 10^{40}$ is unexpectedly related to another dimensionless constant.
- *Which exactly:* the fine structure constant $\alpha \approx 1/137$ from quantum electrodynamics.
- *Chemical meaning:* crudely speaking, the largest possible size of an atom is $1/\alpha$.
- *Dirac's observation:* $10^{40} \approx 2^{1/\alpha}$.
- *Caution:* this is not an exact equality but, on the other hand, we do not even know T well enough.
- *Why?* no good explanation is known.

9. Feynman's 1985 Opinion

- According to R. Feynman, the value $1/\alpha$

  "has become a mystery ever since it was discovered more than fifty years ago, and all good theoretical physicists put this number up on their wall and worry about it. Immediately you would like to know where this number for a coupling comes from. Nobody knows. It is one of the *greatest* damn mysteries of physics: a *magic* number that comes to us with no understanding by man"

- *Our claim:* simple cognizability (= computational complexity) arguments can explain this value.
- *Caution:* we cannot explain the *exact* value of α, since T is only approximately known.
- *We hope:* that physicists will start looking for more serious quantitative explanations.

10. Our Back-of-the-Envelope Explanation: Assumptions

- *Fact:* to describe a state of an n-particle cluster, we must know,
  - for each combination of coordinates $(\vec{x}_1, \ldots, \vec{x}_n)$,
  - the value of the wave function $\Psi(\vec{x}_1, \ldots, \vec{x}_n)$.
- *Reasonable assumption:* the world is cognizable.
- *In other words:* we must be able to predict at least something for such n-particle clusters.
- *Question:* from this viewpoint, what is the largest size n of the atom.
- *In other words:* what is the largest size of the cluster of actively interacting particles?

11. Predict ''Something'': What Does that Mean?

- *Our assumption:* we can predict *something* about the location of each of n particles.
- *What it does not mean:* that we can predict *everything* about the locations of all n particles.
- *The smallest possible amount of information:* when we know exactly one bit of information.
- *What is a bit:* an answer to a "yes"-"no" question.
- *In other words:* we ask one question about the location and get the answer "yes" or "no".
- *Formalization:* for each particle i, let S_i^+ be the set of all the locations in which the answer is "yes".
- *Conclusion:* the "no" set is $S_i^- = -S_i^+$.

12. Analysis of Computational Complexity

- *Case of a single particle:* we must know two probabilities:
  - the probability $\int_{\vec{x}\in S^+} \rho(\vec{x}\,)\,\mathrm{d}\vec{x}$ that the particle is located in the set S^+, and
  - the probability $\int_{\vec{x}\in S^-} \rho(\vec{x}\,)\,\mathrm{d}\vec{x}$ that the particle is located in the set S^-.
- *General case of n particles:* we want to describe, for each particle i, whether $\vec{x}_i \in S_i^+$ or $\vec{x}_i \in S_i^-$.
- *We must describe:* for each possible combination of sets $S_i^\pm$, what is the corresponding integral probability.
- *Counting:* there are exactly 2^n possible combinations $(S_1^\pm, \ldots, S_n^\pm)$.
- *Conclusion:* we must know at least 2^n different probabilities.

13. Derivation of Dirac's Relation

- *Reminder:* we must know at least 2^n different probabilities.
- *Corollary:* we must consider at least 2^n different values of the corresponding wave function $\Psi(\vec{x}_1, \ldots, \vec{x}_n)$.
- *Fact:* our prediction algorithm must handle each of 2^n values at least once.
- *Conclusion:* this algorithm should require at least 2^n computational steps.
- *Fact:* during the entire history of the Universe, we can perform no more than $T/\Delta t$ computational steps.
- The largest possible atom is thus the one for which we need this largest number of steps: $2^n \approx T/\Delta t$.
- This is exactly Dirac's relation.

14. Caution

- The above derivation is a "first approximation", back-of-the-envelope calculation.
- In reality, the situation is more complicated.
- *On the one hand:* we can speed up computations if we use quantum or parallel computation.
- Then, in time $T/\Delta t$, we can perform $> T/\Delta t$ computational steps.
- *On the other hand:*
  - to predict whether in the future, $\vec{x}_i \in S_i$ or not,
  - it is not enough to know whether $\vec{x}_i \in S_i$ at $t = t_0$.
- As a result, we need to process much more than 2^n units of data.
- It is desirable to lift our qualitative explanation to a more accurate and reliable physical level.

15. Using Under-Utilized Space-Time-Causality Processes for Computation

- *Problem:* computations may take a long time.
- *Explanation:* traditional computational complexity estimates are based on traditional physics and traditional space-time.
- *Known fact:* quantum effects can drastically speed up computations:
  - time needed for search in an unsorted list of size n is reduced from n to $\sqrt{n}$;
  - time needed to factor large large numbers is reduced from exponential to polynomial, etc.
- *Less known fact:* space-time-causality processes can also lead to a drastic computational speed up.

16. Parallelization: Reminder

- *Good news:*
  - parallel computers can speed up computations;
  - the more processors, the faster computations.
- *Analysis:* during the parallel computation time T_p, we can only access computers within a sphere $R = c \cdot T_p$.
- Within this sphere of volume $V = \dfrac{4}{3} \cdot \pi \cdot R^3 \sim T_p^3$, we can only fit $\le V/\Delta V \sim T_p^3$ processors of size ΔV.
- All these processors can perform $T \le T_p \cdot \text{const} \cdot T_p^3 = C \cdot T_p^4$ computational steps.
- *Conclusion:*
  - if a computation requires T sequential steps,
  - we need $T_p \ge C \cdot T^{1/4}$ steps to perform it in parallel.
- *Conclusion:* exponential time is unavoidable.

17. Parallelization in Curved Space-Times

- *Observation:* the above lower bound on parallel computation time depends on the formula $V(R) = \frac{4}{3} \cdot \pi \cdot R^3$.
- *Known:*
  - this formula only holds in Euclidean geometry, and
  - actual space-time is curved (= not Euclidean).
- *Natural idea:* we may get faster parallel computations in curved spaces.
- *Known:* in Lobachevsky space,

$$V(R) = 2\pi k^3 \cdot \left(\sinh\left(\frac{R}{k}\right) \cdot \cosh\left(\frac{R}{k}\right) - \frac{R}{k} \right) \sim \exp\left(\frac{2}{k} \cdot R\right).$$

- *Corollary:* we can fit exponentially many processors into a sphere of radius $R = c \cdot T_p$.
- *Conclusion:* in Lobachevsky space, parallelization can reduce exponential time $T = 2^n$ to linear time $T_p \sim n$.

18. Parallelization in Curved Space-Times (continued)

- *Good news:* in Lobachevsky (constant curvature) space, parallelization speeds up computations.
- *Problem:* actual space-time is more complex.
- *Good news:* there exist more realistic space-time models with the same property.
- *Known:* there is no way to escape from a black hole.
- *Known:* as the matter collapses, the escape throat gets narrower.
- *Less known:* there exist "almost" black hole models.
- *Clarification:* models with a throat so narrow that they look like elementary particles.
- *Known hypothesis:* particles are such "almost" black holes, entering into other "universes".

19. Parallelization in Curved Space-Times: Proposal

- *General problem:* we must find an object x that satisfies a certain property $F(x)$.
- *In the computer:* everything is represented as a sequence $x = (x_1, \ldots, x_n)$ of 0s and 1s ("binary string").
- *Computer description:* given a property $F(x)$, find a binary string x that satisfies this property.
- *How to solve it:* to find $x = (x_1, \ldots, x_n)$, $x_i \in \{0, 1\}$ such that $F(x)$, we:
  - find two particles (and corr. worlds);
  - ask World 1 to search for $x = (0, x_2, \ldots, x_n)$ s.t. $F(x)$;
  - ask World 2 to search for $x = (1, x_2, \ldots, x_n)$ s.t. $F(x)$.
- Each of these worlds does the same split w.r.t. x_2, etc.; in time $2n$ ($\ll 2^n$), we get an answer back.

20. Another Idea: Using Hypothetic Acausal Processes

- *Known fact:* several physical theories have led to micro- and macro-causality violations, i.e., going back in time.
- *Feynman:* positrons are electrons going back in time.
- *Mainstreaming:* K. Thorne's Physical Reviews papers.
- *General relativity:* space-time generated by a massive fast-rotating cylinder contains a closed timelike curve.
- *String theory*: interactions between string-like particles sometime lead to the possibility to influence the past.
- *Cosmology:* a short period of exponentially fast growth ("inflation") can lead to a causal anomaly.

21. Paradoxes of Acausality

- *Paradox of causality violation:*
  - a time traveler goes into the past and kills his father
  - before he himself was conceived.
- *Solution:* since the time traveler was born, some unexpected event prevented him from killing his father.
- The time traveler takes care of all such probable events.
- *But:* there are always events with small probability which cannot all be avoided.
- *Example:* a meteor falling on the traveler's head.

22. Using Acausal Processes for Computations

- *Example:* propositional satisfiability problem with n variables.
- *Straightforward option:* computer computes and send result back in time, to us now.
- *Problem:* with time travel, we may invoke an event with a very small probability $p_0 \ll 1$, and ruin computations.
- *Alternative algorithm:*
  - generate n random bits $x_1, \ldots, x_n$ and check whether they satisfy a given formula F;
  - if not, launch a time machine that is set up to implement a low-probability event.

23. Using Acausal Processes for Computations: Analysis

- *Algorithm* (reminder):
  - generate n random bits $x_1, \ldots, x_n$ and check whether they satisfy a given formula F;
  - if not, launch a time machine that is set up to implement a low-probability event.
- *Analysis:* nature has two choices:
  - generates n variables which satisfy the given formula (probability 2^{-n}),
  - time machine is used, triggering an event with probability p_0.
- If $2^{-n} \gg p_0$, then the first event is much more probable.
- So, the solution to the problem will actually be generated (without the actual use of a time machine).

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