From the Nine Muses and Four Elements to RealQM and AI

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Abstract

The Greeks sought to understand the world through a few fundamental constituents interacting through a few universal principles. Empedocles named four elements and two forces, Love and Strife. This essay follows that programme through the history of physics to Real Quantum Mechanics (RealQM), in which electrons are charge densities in three-dimensional space interacting through Coulomb's law, and asks whether AI, by taking over the solution of equations, may return physics to its first question: what is a physically meaningful model of reality?

1 The Muses and the elements

The ancient Greeks approached both the human mind and the physical world through a small number of fundamental concepts. The nine Muses represented the forms of intellectual and artistic activity: Calliope of epic poetry, Clio of history, Erato of love poetry, Euterpe of music, Melpomene of tragedy, Polyhymnia of sacred song, Terpsichore of dance, Thalia of comedy—and Urania of astronomy [1]. That astronomy had its own Muse says something important: science was part of human culture, not a separate technical enterprise, and understanding nature was bound up with the perception of beauty, harmony and order.

2 Empedocles: four roots and two forces

Around 450 BC Empedocles of Akragas in Sicily proposed that everything is composed of four *roots*—the word *element* came later—namely earth, water, air and fire. Their mixing and separation are governed by two opposing principles:

- **Love** (*Philotes*), which brings things together;
- **Strife** (*Neikos*), which drives them apart [2, 3, 4].

This is a remarkably modern form of physical theory: a few fundamental constituents, interacting through universal principles, generate the immense diversity of the observable world. Empedocles wrote his theory as a poem and invoked the Muse Calliope to assist him [2]. Physics, philosophy and poetry were still one enterprise.

3 Love and Strife as gravitation and Coulomb interaction

In the physical world envisaged by RealQM two interactions take centre stage:

- **Gravitation**: attraction between masses;
- **Coulomb interaction**: attraction between opposite charges, repulsion between equal ones.

Gravitation is Love in its purest classical form: it gathers matter into planets, stars and galaxies. Coulomb interaction carries both principles. The attraction between positive nuclei and negative electrons brings matter together; the repulsion between charges of equal sign counteracts unlimited concentration and organises matter in space. Together with wave dynamics, this interplay of attraction and repulsion produces the structures of atoms, molecules and condensed matter.

Both laws are inverse-square laws [5, 6], and both can be written as Poisson equations in three-dimensional space,

$$\Delta\phi = 4\pi G\rho_{\text{mass}}, \qquad -\Delta V = 4\pi\rho_{\text{charge}},$$

so that across 2,500 years there is a conceptual line from Love and Strife to gravitation and Coulomb interaction. It is not a literal identification, but a shared vision of nature organised by a few universal principles of interaction.

4 Strife has two faces

Recent computation adds a twist that Empedocles might have enjoyed. Coulomb repulsion is not the whole of Strife.

Take two helium atoms. Each is a closed shell: two electrons of opposite spin forming a tight pair. In nature two helium atoms brought close repel each other; there is no He_2 molecule in the ordinary sense. In the basic form of RealQM, where electron domains meet at free walls, the computation instead finds a false bond of about half a hartree at a separation of two bohr [22]. Coulomb repulsion between the electron clouds is present, but it is not enough.

What is missing is the other face of Strife: *exclusion* [9]. Two electrons of the same spin cannot occupy the same region of space. In RealQM this is not an abstract symmetry of a wave function but a spatial fact: electrons of the same spin meet at a wall, and the wall must carry a cost—the energy of the part of the electron's density that the wall cuts off. With that cost, set by the electron's own energy and nothing fitted, the false bond disappears and helium repels as it should. The same holds for two beryllium atoms.

So in RealQM Love is Coulomb attraction, and Strife comes in two forms: Coulomb repulsion between charges, and exclusion between electrons of the same spin. Both are statements about matter in three-dimensional space.

5 From Empedocles to modern physics

The history of physics can be read as a sequence of attempts to carry out the programme of Empedocles:

- Democritus: atoms and the void;
- Newton: matter interacting through gravitation;
- Maxwell: electric and magnetic fields [7];
- Einstein: space, time, matter and energy;
- Schrödinger: matter described by wave mechanics [8];
- the Standard Model: elementary particles and quantum fields.

Modern physics recognises four fundamental interactions: gravitation, electromagnetism, and the strong and weak nuclear interactions. RealQM, with its proposed extensions to nuclear physics and cosmology, explores a more economical programme built on gravitation and Coulomb interaction [21]. Whether such a reduction can account for the full range of observed phenomena is an open scientific question.

6 Standard quantum mechanics: simplicity lost?

Standard quantum mechanics (stdQM), originating with Schrödinger in 1926, gives a formally compact description of atoms and molecules. But the wave function of N electrons depends on $3N$ spatial coordinates, not on the three coordinates of physical space. Its direct numerical representation requires resources growing exponentially with the number of electrons—Kohn's "exponential wall" [12]— and a century after its introduction the physical meaning of a function on $3N$-dimensional configuration space remains disputed.

This is a striking contrast to the programme of Empedocles: a formally simple equation produces a representation of nature of enormous computational complexity.

Density functional theory (DFT) [10, 11] brings the computation back to three dimensions, and it is today the workhorse of chemistry and materials science. But it does so by collecting everything that cannot be computed into one unknown term, the exchange–correlation functional, which is defined through the $3N$-dimensional wave function and is in practice a chosen formula. DFT's own leading developers note that there is no systematic way to improve these formulas, and that some fitted to energies have drifted away from the physics [13, 14]. DFT gives good numbers; it does not claim that its objects are physical. It is a three-dimensional computational method for a theory posed in $3N$ dimensions.

7 Density functional theory: saving the phenomena

The theorem. DFT is presented as resting on the Hohenberg–Kohn theorem [10]: the ground-state energy is a functional of the electron density alone, so that DFT is "exact in principle". The argument is a one-line contradiction. Suppose two different external potentials gave the same ground-state density; apply the variational principle to each ground state and add the two inequalities, and one obtains $E_1 + E_2 < E_1 + E_2$. Later work by Levy and Lieb [15, 16] repaired its technical assumptions, and as mathematics it stands.

But the argument uses only two things: that the ground state minimises the energy, and that the external potential enters linearly, as $\int v\rho$. It uses nothing of the kinetic energy, of the Coulomb interaction between electrons, of the number of electrons, or of three-dimensional space. It therefore holds unchanged for *any* interaction between the particles—Coulomb, any

other law, or none. A statement that holds whatever the interaction cannot say anything about the effects of this one. It is an existence statement reached by contradiction: it shows that a functional exists and says nothing about what it is or how to compute it. Everything DFT must actually get right—how electrons avoid each other, exchange, correlation, binding—lies in the exchange–correlation functional, about which the theorem is silent. That functional is defined through the $3N$-dimensional Schrödinger equation and cannot be computed without solving it. An exact theory that cannot be computed makes no prediction and cannot be tested; what is tested is always one of the chosen formulas.

What the theorem does. Its roles are four, and only the first is pure prestige. It gave the density approach a mathematical warrant, and with it respectability in physics: no longer a crude model in the line of Thomas and Fermi, but "exact in principle". It gave permission to seek functionals of the density. It supplies a target: exact properties of the defined functional (its scaling, its limits) are used to constrain approximations such as PBE [17]. And it underlies the Kohn–Sham construction [11], whose fictitious non-interacting electrons reproduce the density and carry the kinetic energy. The physics DFT does contain—kinetic energy, the attraction of the nuclei, the classical Coulomb energy of the density—is taken over from the Schrödinger equation; the many-electron physics that remains is supplied by formulas, chosen by model systems, by imposed constraints, or by fitting to molecular data [18].

History bears this out. Chemists adopted DFT broadly in the 1990s, some thirty years after the theorem, when gradient-corrected and hybrid functionals began to give useful accuracy. Adoption followed the numbers, not the theorem. Kohn's Nobel Prize of 1998 was in chemistry, shared with Pople for computational methods: DFT was honoured as a method, not as physics. The usual presentation has the order reversed: the theorem is offered as the foundation and the approximations as an unfortunate necessity, whereas the approximations carry all the content and the theorem supplies reassurance.

A classical analogue. The fair classical analogue is not dogma: a scripture is accepted on authority and cannot be refuted, while DFT's formulas are tested against measurement every day and their failures are published by their own developers. The analogue is Greek astronomy and its explicit doctrine of *saving the phenomena* [19]. An astronomical model did not need to be physically true; it had to reproduce the observed positions of the planets. Ptolemy's circles were calculating devices, not the mechanism of the heavens, and every new discrepancy was met by adjusting the devices. DFT practises the same astronomy. Its Kohn–Sham orbitals are declared fictitious, as the circles were; its functional is judged by whether it reproduces energies and geometries; new failures are met by new functionals, and there are now hundreds; and a mathematical warrant, the Hohenberg–Kohn theorem, supplies the legitimacy that the doctrine of perfect circles once gave.

A modern analogue, from fluid mechanics, has the same structure. Averaging the Navier–Stokes equations leaves an unknown term, the Reynolds stress, exactly defined by the full equations and uncomputable without solving them; it is modelled by closures with fitted constants, of which there is likewise a zoo. DFT's exchange–correlation term is the Reynolds stress of quantum chemistry.

In 1609 Kepler called his *Astronomia Nova* a *physica coelestis*, a celestial physics [20]: he sought the causes of the planetary motions, not only their positions. His ellipses were at first no more convenient than the established tables, but they were physics, and Newton could build on them. RealQM takes Kepler's side: a model offered as physical, accepting worse numbers for the present in exchange for errors that point to causes. The analogy concerns

method, not truth. Ptolemy's cosmos was false, whereas the Schrödinger equation behind DFT is not known to be wrong: DFT saves the phenomena of a correct but uncomputable theory. But saving the phenomena is what it does.

8 RealQM: recovering the simplicity of nature

Real Quantum Mechanics (RealQM) [21] is an attempt to recover the original ambition of natural philosophy with the means of modern computational mathematics. In RealQM:

- electrons are charge densities distributed in three-dimensional physical space;
- electrons occupy non-overlapping domains with free, moving boundaries;
- electrons and nuclei interact through Coulomb attraction and repulsion, each electron with the others but not with itself;
- atomic and molecular dynamics are governed by time-dependent partial differential equations in physical space.

Instead of one wave function in $3N$ dimensions, an N-electron system is represented by N interacting three-dimensional densities. The computational work can then grow essentially linearly with the number of electrons, given suitable algorithms.

Every object in RealQM is offered as physical, and every approximation is a statement about how electrons behave. That makes the model testable piece by piece. When the basic model bound two helium atoms, the failure pointed to one specific claim—that a wall between electrons costs nothing—and the correction was a physical rule. This is the difference between a model of physics, whose wrong numbers point to the physics that is missing, and a model for numbers, which can be refitted indefinitely without teaching anything about nature. The first is science in the sense of Empedocles; the second, however useful, is closer to Ptolemy's epicycles.

RealQM's present numbers are honest rather than final. For simple molecules its bond lengths are within a few per cent of experiment, at the level of the simplest density functionals, while its binding energies are still off by tens of per cent [22]. The validity of the programme must be settled by computation and comparison with observation.

In the broader picture Coulomb interaction organises matter on the small scale and gravitation on the large. From molecules to galaxies, nature would be understood as matter in physical space, interacting through two laws.

9 AI and the revival of natural philosophy

AI adds a new dimension to this story. Mathematical modelling of the world has three steps:

1. formulating a question about the world;
2. expressing it in a mathematical model;
3. solving the resulting equations.

AI is rapidly transforming the third step and increasingly assists with the second. This may shift the attention of physics back to the first and most fundamental question: *what is a physically meaningful mathematical model of reality?*

The challenge is then not only to solve the equations of stdQM more efficiently, but to ask whether other equations give a simpler, more transparent and more computable description of the physical world. AI makes it possible to explore and test such alternatives at a pace that was unthinkable a few years ago: the work on RealQM reported above—testing a hypothesis, finding where it fails, locating the missing physics and testing the correction—was carried out in a dialogue between a human and an AI.

10 Back to the nine Muses

The nine Muses remind us that understanding involves not only logic and calculation but imagination, intuition, beauty and creativity. Empedocles reminds us that the ambition of physics is to explain the complex through the simple. Newton and Coulomb gave attraction and repulsion precise mathematical form; RealQM seeks to build on these laws through computational models in physical space; and AI may now provide the means to explore that vision on an unprecedented scale.

Could the era of AI bring a renaissance of natural philosophy, uniting physical intuition, mathematical modelling and computational exploration? Could RealQM be a step in that direction?

After 2,500 years the vision of Empedocles remains remarkably attractive: the immense complexity of the world emerging from a few constituents interacting through Love and Strife.

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