

Charge Densities in Real Space: RealQM and the Realist Quest Carried by Schrödinger

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Abstract

The central question of realism in atomic physics is whether the microscopic world is of the same form as the macroscopic — extended matter in ordinary three-dimensional space, only of smaller size — or is something categorically other. Schrödinger’s wave mechanics began as a bet on the first answer, reading $\psi\bar{\psi}$ as a real charge density in space; the Bohr–Born–Heisenberg–Dirac program settled on the second, and the realist reading was set aside. RealQM takes up Schrödinger’s quest. We compare the ontology of an atomic system of N electrons under two models. Standard quantum mechanics treats the electrons as *identical particles* and represents the system by a probability amplitude over their configurations in a $3N$ -dimensional configuration space, antisymmetric under exchange. *RealQM* represents it by N unit charge densities, each carried on its own region Ω_i of ordinary three-dimensional space, the regions non-overlapping ($\Omega_i \cap \Omega_j = \emptyset$). Two long-standing metaphysical problems — the *arena* of the wave function and the *individuality* of identical particles — attach to the first model, one to each of its two features: the $3N$ -dimensional domain and the antisymmetry. The second model has neither feature and so incurs neither problem. It is a primitive ontology in three-space (no configuration-space object exists), and it *individuates* its electrons absolutely, by the regions they occupy (the Principle of the Identity of Indiscernibles is satisfied); the two virtues are one fact, the non-overlap of the Ω_i doing double duty. We then argue that the decisive asset is computational: the standard amplitude is intractable beyond very small N , forcing every practical method to retreat from the $3N$ -dimensional object toward effective three-dimensional ones (density-functional theory makes the three-dimensional density fundamental in practice), whereas in RealQM the three-dimensional charge densities *are* the objects of computation, and the same functional has been used to compute atoms across the periodic table, molecular bonds and hydrogen bonds, and — reading the nucleus as protons and electrons bound by Coulomb alone — nuclear binding energies. The metaphysics is thus not posited for interpretive tidiness but carried by a working, empirically tested method. We place the proposal against the point-particle ontology of the Standard Model, answer the main objections, and bound the claim.

1 Introduction: the realist question and Schrödinger’s quest

The central question of realism in atomic physics can be put in one line: *is the microscopic of the same form as the macroscopic — extended matter in three-dimensional space, only of smaller size — or is it categorically other?* On the first answer an atom is a small physical object of the same kind as a large one, picturable in ordinary space; on the second it is not a thing in space at all

but an element of an abstract formalism whose only contact with space is through the statistics of measurement.

Wave mechanics began on the first side. In 1926 Schrödinger read the wave function of an electron as a continuous distribution of electric charge in ordinary space, $\rho = e\psi\bar{\psi}$, and sought an *anschaulich* — intuitive, visualizable — account of atomic phenomena in terms of such extended waves, in deliberate opposition to the unvisualizable discontinuities of the older quantum theory [1, 3]. On this reading an atom is a standing charge-density pattern in three-space: a picture one can draw, of the same form as a macroscopic charge distribution, only atomic in size.

Within a year the realist reading was displaced. Born recast $\psi\bar{\psi}$ as a probability density [2]; Heisenberg’s matrix mechanics and uncertainty relations, Bohr’s complementarity, and Dirac’s abstract transformation theory turned the formalism into an instrument for computing measurement probabilities rather than a picture of what there is. Decisive for our purposes is *why* the charge-density reading had to go: for N electrons the wave function lives not on ordinary space but on a $3N$ -dimensional configuration space, where it cannot be a charge density in $\mathbb{R}^3$. *Anschaulichkeit* was surrendered at exactly the point where the domain left three-space — the answer to the realist question turned on the arena of the wave function.

RealQM [22] takes up the abandoned quest. It is a reformulation of the Schrödinger equation for atomic physics that keeps Schrödinger’s charge densities in ordinary three-space, but resolves the many-electron system into N *separate* unit densities on non-overlapping regions, so that the charge-density realism which failed on $\mathbb{R}^{3N}$ becomes viable again on $\mathbb{R}^3$. It is, potentially, a revolutionary change of formulation: the same atomic, molecular, and nuclear physics, computed and visualized as extended charge in real space, microphysics of the same form as macrophysics. This paper sets out its ontology, asks what philosophy gains from it — two classic problems dissolved together (§§2–4) — and asks what keeps it from being one more homemade picture: that it computes (§5).

2 Two problems in one formula

An atomic system of N electrons admits two descriptions. Standard quantum mechanics treats the electrons as *identical particles* and represents the system by one probability amplitude over their joint configurations, in a space of $3N$ dimensions. RealQM [22] treats them as N *individual charge densities*, each carried on its own region $\Omega_i \subset \mathbb{R}^3$, in ordinary three-dimensional space (§3). This contrast — identical particles in a high-dimensional configuration space against individuated densities in ordinary space — is the whole of what follows. We take the standard side first.

Write its state:

$$\Psi : \mathbb{R}^{3N} \rightarrow \mathbb{C}, \quad \Psi(\dots, \mathbf{x}_i, \dots, \mathbf{x}_j, \dots) = -\Psi(\dots, \mathbf{x}_j, \dots, \mathbf{x}_i, \dots). \quad (1)$$

The domain is $\mathbb{R}^{3N}$; the minus sign is the *antisymmetry* of the amplitude under exchange of any two particles — Fermi–Dirac statistics, the Pauli principle in its formal guise. Two metaphysical difficulties follow directly, one from each of these two features of (1).

The arena, from the domain $\mathbb{R}^{3N}$. If Ψ is the fundamental object — wave-function realism [6, 7, 8] — then ordinary three-space is not fundamental but must be recovered from a field on a $3N$ -dimensional space, and the manifest world of things in space becomes a derived appearance. The rival *primitive ontology* programme [9, 10, 11, 19] insists instead on beables in $\mathbb{R}^3$ — particles, a matter density, or flashes — with Ψ demoted to a dynamical or nomological role. A middle route, *spacetime state realism*, keeps a description in spacetime by assigning density operators to

its regions [18], yet the fundamental state remains the global, entangled one and separable objects in $\mathbb{R}^3$ are not thereby recovered. Either way the $3N$ -dimensional domain is the source of the difficulty: one must swallow it as fundamental, explain it away, or relocate it.

Individuality, from the antisymmetry. The permutation symmetry in (1) makes the particles, on the received reading, *non-individuals*: no fact settles which is which, and two electrons in one atom are numerically distinct yet share all state-dependent and state-independent properties, in apparent violation of Leibniz's Principle of the Identity of Indiscernibles (PII) [12, 13]. Defenders of PII have retreated to *weak discernibility* by symmetric irreflexive relations, conceding that no distinguishing *monadic* property is available [14, 15]. Later work has refined the taxonomy of (in)discernibility and pressed it in both directions [16, 17], but on no variant does an electron in a many-electron state carry a distinguishing *monadic* property.

Both problems are consequences of the two choices in (1): the domain $\mathbb{R}^{3N}$, and the antisymmetry. A formulation making neither choice does not incur them.

3 A real-space ontology, in equations

Take instead the RealQM formulation [22]

$$\Psi(\mathbf{x}) = \sum_{i=1}^N \psi_i(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3, \quad \text{supp } \psi_i = \overline{\Omega_i}, \quad \Omega_i \cap \Omega_j = \emptyset \ (i \neq j), \quad (2)$$

where ψ_i^2 is the unit charge density of electron i on its own region $\Omega_i \subset \mathbb{R}^3$ and $\rho = \sum_i \psi_i^2$ is the total electron density. For a nucleus (kernel) of charge Z at the origin, with attractive potential $V(\mathbf{x}) = Z/|\mathbf{x}|$, the ground state minimises the energy

$$E = \sum_i \frac{1}{2} \int_{\Omega_i} |\nabla \psi_i|^2 - \int V \rho \, dx + \frac{1}{2} \iint \frac{\rho(x)\rho(y)}{|x-y|} \, dx \, dy, \quad \int_{\Omega_i} \psi_i^2 \, dx = 1, \quad (3)$$

over the ψ_i and the free boundaries $\partial\Omega_i$, which meet in Bernoulli (zero-flux) contact conditions. The Pauli principle enters not as an antisymmetry of a function but as the geometric requirement that the Ω_i do not overlap.

RealQM is, at once, a *primitive ontology in three-space*: what exists is the extended charge density ρ in $\mathbb{R}^3$, resolved into the N pieces ψ_i^2 , and there is *no* object on $\mathbb{R}^{3N}$ to interpret or to recover three-space from — (1)'s domain is simply absent. Unlike primitive-ontology theories that carry a matter density *alongside* a configuration-space Ψ that still does the dynamical work [10], here the density is the whole matter ontology and (3) is its law: there is no second, higher-dimensional object in the theory at all. It is a rival theory, not a reinterpretation of (1), and its warrant is the chemistry and nuclear structure it computes (§5).

4 Individuation by occupation

The basic objects of (2) are extended and disjoint, and this individuates them. Define electron i as the density on Ω_i ; then occupancy of Ω_i is a *monadic* property that i has and $j \neq i$ lacks, since $\Omega_i \cap \Omega_j = \emptyset$. Hence

$$i \neq j \iff \Omega_i \neq \Omega_j : \quad \text{no two electrons share all properties.} \quad (4)$$

The Principle of the Identity of Indiscernibles, standardly taken to fail for (1), is *satisfied*. Moreover the electrons are *absolutely* discernible — each has a distinguishing monadic property, the region it occupies — which is stronger than the *weak* discernibility by relations [15] to which PII’s defenders retreat under (1). Individuality in the full classical sense, with a haecceity grounded in a spatial fact rather than a primitive thisness, is recovered.

Extension and individuation are here *the same fact*. The disjointness $\Omega_i \cap \Omega_j = \emptyset$ that keeps each ψ_i a density in $\mathbb{R}^3$ (the primitive-ontology virtue) is the very disjointness that discerns the electrons (the individuality virtue). Where (1) encodes exclusion as antisymmetry — a fact about a configuration-space function — (2) encodes it as impenetrability, a fact about *space*: two charge clouds cannot occupy one place. Pauli exclusion and the identity of indiscernibles, distinct and even opposed in the received picture, are one geometric fact here.

5 Computation: where the ontology earns its weight

A metaphysics can be clean and still idle. What keeps the present proposal from being one more homemade picture is that its ontology is also a working computational method, and one that sits closer to the actual practice of quantum chemistry than the official $3N$ -dimensional ontology does.

The dimensional wall. The amplitude (1) lives on $\mathbb{R}^{3N}$, and representing it there costs exponentially in the number of particles: a modest grid of m points per axis needs m^{3N} values, so solving (1) directly is feasible only for very small N . Essentially all of computational quantum chemistry is a response to this wall. Hartree–Fock replaces Ψ by a single antisymmetrised product and solves in $\mathbb{R}^3$; post-Hartree–Fock methods add back correlation at steep cost; and density-functional theory, by the Hohenberg–Kohn theorems [20, 21], proves that the ground-state energy is a functional of the *three-dimensional* density $\rho(\mathbf{r})$ alone and computes with that object, not with the $3N$ -dimensional amplitude. The overwhelmingly used methods thus already retreat from configuration space to effective three-dimensional quantities. The $3N$ -dimensional object is where the metaphysics is placed but not, for many electrons, where the computation is done.

RealQM computes with its beables. In (2)–(3) the beables *are* the objects of computation. One minimises the energy (3) directly over the charge densities ψ_i and their free boundaries in $\mathbb{R}^3$; complexity scales with mesh points in three dimensions, not with the exponential dimension of $\mathbb{R}^{3N}$. Where density-functional theory makes the three-dimensional density fundamental as a *calculational* device while leaving the $3N$ -dimensional Ψ as the official ontology, RealQM takes the three-dimensional densities to be fundamental *full stop*, and reads (3) as the law they obey. The ontology is not supplied after the calculation, as an interpretation of a formalism solved elsewhere; it is what one computes with. An ontology that is also the algorithm is answerable to computation in a way a pure interpretation is not.

The empirical record. The functional (3), with the appropriate kernels, has been applied across a wide range of systems as a single method, not tuned per case [22, 23, 28]:

- *Atoms.* Ground-state energies computed across the periodic table by direct free-boundary minimisation, with shell structure emerging from the packing of the Ω_i rather than from imposed antisymmetry [23].

- *Molecules.* Covalent bonds, molecular geometries, and hydrogen-bonded complexes; for water the computed dipole moment comes out near the experimental value, and hydrogen-bond energetics are reproduced [22, 28].
- *Nuclei, by Coulomb alone.* Read as protons and electrons bound by the same electrostatic energy (3) at femtometre scale — with no strong or weak force — the model returns nuclear binding energies of the right size: the ${}^4\text{He}$ binding comes out close to experiment, and the ratio of ${}^4\text{He}$ to deuteron binding is reproduced to within a few percent [24, 25]. The same Coulomb picture describes fusion as a rearrangement of protons and electrons [26].

These are not paper derivations but a public library of interactive, browser-runnable simulations [28] in which the charge densities of atoms, molecules, reactions, and nuclei can be computed and watched directly, and several of the results are set out in companion papers under review [23, 24, 25, 26].

Computing the world is evidence of tracking it. That a single, parameter-poor functional reproduces observations across such disparate regimes — atomic ground-state energies, molecular geometry and hydrogen bonding, nuclear binding by Coulomb alone — spanning length scales that differ by some five orders of magnitude, is not interpretive bookkeeping but hard empirical evidence. A model free to fit one regime by adjustment is cheap; a model that computes many *independent* regimes at once, under the same law (3) and with no per-case tuning, is expensive to fake. On the familiar no-miracles reasoning, such consilience is a strong sign that the model has latched onto real structure rather than onto an artefact of representation — and here that structure just is the ontology of §3: extended charge in three-space obeying (3). Behind this lies a realist principle worth stating plainly: *what is real is computable*. The ground is the character of physical process itself. Nature runs as an analog computation — physical states evolving in real space under physical law — and an analog process of this kind can be expected to be reproducible in digital form, by a finite constructive procedure, provided the mathematical model used expresses the real physics rather than an artefact of representation. Digital computability is thus the expected signature of a model that captures what the world actually does, and persistent intractability a warning that a model carries structure the world does not. On the realist reading nature’s analog computation is moreover carried out *in three-dimensional space*, on charge and field — not in a $3N$ -dimensional configuration space — so a model formulated in $\mathbb{R}^3$ shares the very substrate on which the world computes. That is why RealQM is directly computable there, just where the $3N$ -dimensional amplitude is not: the tractability gap tracks the difference between a model that expresses the real physical process and one laden with representational overhead. RealQM earns its ontology by computing what nature computes, in the space where nature computes it; it is on that record, not on interpretive convenience, that the metaphysics of §§3–4 rests.

6 The point and the field: a perspective

The extension at issue reaches past non-relativistic quantum mechanics. The Standard Model’s Lagrangian carries three gauge forces together with a Higgs and Yukawa sector,

$$\mathcal{L}_{\text{SM}} = -\frac{1}{4}F_{\mu\nu}^a F^{a\mu\nu} + \bar{\psi} i\gamma^\mu D_\mu \psi + |D_\mu \Phi|^2 - V(\Phi) - (y \bar{\psi}_L \Phi \psi_R + \text{h.c.}), \quad (5)$$

its fundamental carriers *point* excitations of quantum fields. That is a second departure from *res extensa*: where (1) moved the object into $\mathbb{R}^{3N}$, field theory shrank it to a point in $\mathbb{R}^3$. The point carries the classical infinity of a zero-extension charge’s self-energy, softened but not cured by renormalisation — and it is telling that string theory restores extension (to strings) precisely to tame it. Retaining only the electromagnetic term of $\mathcal{L}_{\text{SM}}$ and reading it, non-relativistically and electrostatically, as extended densities returns the energy functional (3): RealQM is, in this sense, that one term read as *res extensa* in $\mathbb{R}^3$ [27]. The ontological choice — the point or the extended thing — is thus one question asked at every scale, and RealQM answers it, in its domain, on the side of extension. Nothing here disputes the Standard Model’s quantitative account of sub-nucleonic phenomena; the claim is about which ontology one reads off the electromagnetic sector at atomic and nuclear scale.

7 Objections and replies

Non-overlap is ad hoc. *Objection:* imposing $\Omega_i \cap \Omega_j = \emptyset$ is a stipulation put in to get individuation for free. *Reply:* it is the geometric form of the Pauli principle, and it is what the free-boundary minimisation of (3) actually enforces — the domains and their boundaries are solved for, not drawn by hand. That the same condition also individuates is the content of §4, not an extra assumption: one fact, read twice.

What about interference and entanglement? *Objection:* the power of (1) is that it captures superposition and entanglement, which a sum of disjoint densities seems to lose. *Reply:* this marks the scope of the claim. RealQM is offered as an ontology and computational model for *stationary bound states* — the ground and excited states of atoms, molecules, and nuclei — where it is tested [22, 23, 24]. Time-dependent and multi-centre phenomena are treated by a complex, current-carrying extension of the same real-space formulation [22]; whether that extension recovers the full range of interference effects is open and is flagged as such (§9). The metaphysical thesis here concerns the bound-state regime, and is conditional on empirical adequacy there.

Is computability a metaphysical virtue at all? *Objection:* tractability is pragmatic, not ontological; a theory is not truer for being easier to compute. *Reply:* the point is not ease but *answerability*. In RealQM the posited beables are the very quantities carried through the calculation and compared with experiment, so the ontology is directly exposed to empirical test; in the interpretive programmes the beables are added to a formalism that is solved, and confirmed, in terms of other objects. An ontology that does the computing is falsifiable in a way an interpretation grafted onto a shared formalism is not — and that is an epistemic virtue, not merely a convenience.

It is a fringe, self-published programme. *Objection:* the physics is not established in the mainstream literature. *Reply:* granted, and the metaphysical verdict is stated as conditional on that physics (§9). But the conditional is not idle: the computational results exist, are public and reproducible [28], and are set out in papers under review [23, 24, 25]. The philosophical interest is that *if* a real-space charge-density model is empirically adequate in its domain — an open question being pressed — then it resolves the arena and individuality problems together, which is a reason to take the model seriously rather than to dismiss it in advance.

8 A note on dissolution

There is a deflationary way to hear the foregoing that should be met head on. On the reading defended here the arena and individuality problems are not so much *solved* as made to *disappear*: once the fundamental object is extended charge in three-space rather than an amplitude on configuration space, the question of how to recover ordinary space from $\mathbb{R}^{3N}$, and the question of what individuates permutation-symmetric particles, simply do not arise. This is dissolution in Wittgenstein's sense — the problems stand revealed as artefacts of a representation mistaken for the world, and clarity makes them vanish rather than answering them on their own terms [4, 5]. To a philosopher of physics this can disappoint at first: a substantial and ingenious literature has grown around puzzles that the realist reformulation quietly removes.

But the disappointment is only the first step. What the dissolution clears away is a set of problems *internal to a formalism*; what it leaves standing is the harder and more properly physical question of *what reality is* — that it should be extended charge in three-dimensional space, evolving under (3), and computable because the world itself computes (§5). With the classic puzzles gone, the questions that remain are about the thing itself: the time-dependent, current-carrying regime, the status of interference and entanglement under a real-space ontology, and why nature's analog computation takes the form it does. Dissolving the idealist problems is thus not an end but a redirection — from puzzles about our representation of matter to the analysis of the matter represented.

9 Conclusion

The arena of the wave function and the individuality of particles are two readings of the two features of one formula, (1): its $3N$ -dimensional domain and its antisymmetry. RealQM, the real-space charge-density formulation (2)–(3), declines both, and so meets both problems with one move — a primitive ontology in three-space whose electrons are individuated absolutely, by the regions they occupy, because $\Omega_i \cap \Omega_j = \emptyset$ does double duty. Extension and individuation are the same fact, and Pauli exclusion and the identity of indiscernibles coincide. What lifts this above a merely tidy picture is that the ontology is a working, tested computational method: the standard amplitude is intractable beyond very small N and practice already retreats to three-dimensional objects, while RealQM takes those objects as fundamental and computes atoms, molecules, and — by Coulomb alone — nuclei with them [23, 24, 25]. The open questions are real: the time-dependent extension, the full range of interference and entanglement, and the empirical standing of the programme in the mainstream. But the philosophical payoff is sharp and conditional in a well-defined way: whether such a model is empirically adequate is for physics to decide; if it is, its metaphysics is, on these two long-contested points, the cleaner one.

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