RealQM Atomic Spectra
Radiation as Real Charge Oscillation

Claes Johnson[1]

[1]KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden ,
claesjohnson@gmail.com

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Abstract

Atomic spectra were the starting point of quantum mechanics: the discrete lines a classical atom cannot explain. Standard quantum mechanics accounts for a line *formally* — as the beat of a *superposition* of two eigenstates, a device whose physical meaning is the unresolved question of measurement. Real Quantum Mechanics (RealQM), which represents N electrons by N unit charge densities on non-overlapping domains of ordinary three-dimensional space, gives a physical account instead: a line is a real charge density oscillating between two configurations at their energy difference $E_n - E_m$, a dipole resonating with radiation at that frequency — a definite, deterministic motion of charge rather than a formal superposition. The energies are RealQM's own, from a non-overlapping, self-interaction-free functional whose geometric electron-avoidance captures correlation that a single-determinant mean field misses (helium ground state -2.90 Ha, versus Hartree–Fock -2.86 and exact -2.9037). The selection rule becomes geometry: a line radiates when the charge swings to one side (an l-changing, $s \to p$ transition) and is *dark* when the oscillation is spherically symmetric ($s \to s$) — which is exactly the metastability of the $2s$ states. Helium's optical lines come out as one-active-electron transitions in the screened field of the inner core, including the 587.6 nm D_3 line by which helium was discovered in the Sun. The moving charge is a current, so the radiating dynamics is complex-valued — a real, currentless density is static and dark — placing radiation as the *oscillating*-current member of the complex time-dependent family, beside magnetism (circulation) and spin, on which the companion articles build; only the energies are strictly real. What RealQM adds is a physical mechanism together with its own, correlation-improved energies; what it does not reach is the spin (ortho/para) structure.

1 Real-valued RealQM

RealQM [1] represents N electrons by densities ψ_j^2, each on its own region $\Omega_j \subset \mathbb{R}^3$, the regions non-overlapping, the nuclei a fixed kernel of potential $V_{\rm K}$. The wave functions ψ_j are real, of unit charge $\int_{\Omega_j} \psi_j^2 = 1$ and finite kinetic energy, and the total $\Psi = \sum_j \psi_j$ is continuous across the interfaces. The ground state minimises the Coulomb energy

$$E = \sum_j \tfrac{1}{2}\int_{\Omega_j} |\nabla\psi_j|^2 + \int V_{\rm K}\,\rho\,dx + \sum_{j<k}\iint \frac{\psi_j^2(x)\,\psi_k^2(y)}{|x-y|}\,dx\,dy, \qquad \rho = \sum_j \psi_j^2, \tag{1}$$

the electron–electron repulsion running over *distinct* domains only. There is *no self-repulsion*, and the kinetic energy takes over the confining role that would otherwise fall to it. The energy is

minimised over the wave functions alone; the free boundary is an outcome, its position fixed by density continuity and its shape by the natural (Neumann) condition of the minimisation.

Two features matter for what follows. First, the stationary states — the ground state and the excited configurations — are the stationary points of (1), at total energies $E_0 < E_1 < \cdots$; these are the *levels*. Second, because the electrons occupy *separate* domains they physically avoid one another — a real correlation hole built into the geometry, which a single-determinant mean field does not have. RealQM's energies are therefore its own, and can improve on Hartree–Fock: for helium the ground state comes out at -2.90 Ha (against Hartree–Fock -2.86 and exact -2.9037), recovering from geometry alone the correlation the determinant misses. The spectrum is built on these real levels.

2 Radiation as real charge oscillation

The spectrum is the most visible aspect of an atom, yet standard quantum mechanics hides the physics of how it arises: the levels are eigenvalues and the lines transition probabilities, but what *physically* radiates is never said. In RealQM it is a real charge oscillation — a definite motion of charge in space, deterministic, not a formal superposition.

Only energy *differences* are observable — the zero of energy is free, and with it the absolute clock that would carry it. What the charge does — the density — oscillates at the difference. A line is the charge density moving between two configurations n and m,

$$\rho(x,t) = \rho_0(x) + \delta\rho(x)\,\cos\big((E_n - E_m)t\big), \qquad \mathbf{p}(t) = \cos\big((E_n - E_m)t\big) \int \mathbf{x}\,\delta\rho(x)\,dx, \tag{2}$$

a real oscillation with a dipole moment $\mathbf{p}(t)$. This oscillating dipole *resonates* with the electromagnetic field at its own frequency $E_n - E_m$ and radiates, as a classical antenna does. The energies come from the real theory (1); the line sits at their difference, and only differences are observed — the absolute clocks cancel.

That the density *moves* makes this a *current* phenomenon. By charge conservation $\partial_t\rho + \nabla\cdot\mathbf{j} = 0$, a moving density carries a current $\mathbf{j} = \mathrm{Im}(\psi^*\nabla\psi)$, which is *zero for a real* ψ: a real, currentless density is static and *dark*, so the wave function must be complex *during* the transition. Radiation is therefore the *oscillating*-current member of the same family as magnetism (the *circulating* one), built on the complex time-dependent foundation [2]. What is real is the outcome — the levels, and the observed difference-frequency dipole — not the phase that carries the flow.

The contrast with the standard account is where RealQM earns its keep. There a line is written as

$$\Psi = a\,\Psi_n\,e^{-iE_nt} + b\,\Psi_m\,e^{-iE_mt}, \tag{3}$$

the beat of a *superposition* of two eigenstates — a formal object in configuration space whose physical content is left open, what it *is* to be in a superposition of two energy states being the unresolved question of measurement. RealQM reads the same mathematics as a physical event: a real charge cloud sloshing back and forth in three-dimensional space, deterministic, radiating as it goes, with no collapse — a definite motion of charge in place of an abstract amplitude.

3 Selection rules as geometry

By (2) the oscillation radiates only if it carries a net dipole, $\int \mathbf{x}\,\delta\rho \neq 0$. This turns the selection rule into a statement about shape:

- if the two configurations differ in *angular* character — $s \to p$, the cloud swinging to one side — then $\delta\rho$ is lopsided, $\int \mathbf{x}\,\delta\rho \neq 0$, and the line *radiates*;
- if the oscillation is *spherically symmetric* — $s \to s$, the cloud breathing in and out — then $\delta\rho$ is spherical, its dipole vanishes (indeed no radiating multipole survives, only the forbidden monopole), and the line is *dark*.

So "allowed" and "forbidden" become visible: does the charge lean, or merely pulse. And the *metastability* of a dark state is now physical — nothing radiates because nothing swings to one side. The $2s$ states of helium ($2^1S, 2^3S$) are exactly this: their only route to the ground, $1s^2 \to 1s2s$, is $s \to s$, spherical, dark, so they cannot radiate a dipole photon and live orders of magnitude longer than ordinary excited states.

4 Hydrogen and helium

Hydrogen. One electron, one domain, the bare Coulomb field. The $-1/r$ potential carries the accidental l-degeneracy — $2s$ and $2p$ share an energy — so the levels depend on n alone and the spectrum is the single Rydberg pattern. The lines are that electron's cloud swinging between shapes: Lyman-α ($1s \to 2p$, 10.2 eV), Balmer, and the rest, each an l-changing dipole oscillation.

Helium. Two electrons; the inner $1s$ *screens* the $+2$ kernel, so the outer electron sees a non-Coulomb field — $-2/r$ near the nucleus, $-1/r$ far out — and the l-degeneracy is *lifted*: a penetrating $2s$ is more bound than a $2p$. The optical spectrum is therefore a one-active-electron spectrum, the outer electron transitioning in the screened field of the inner core, and RealQM's radial solve reproduces the levels at the observed values. The visible lines follow as l-changing differences:

transition (outer electron)	ΔE	line
$2p \to 2s$	1.14 eV	1083 nm (infrared)
$3s \to 2p$	1.76 eV	706.5 nm (red)
$3d \to 2p$	2.11 eV	587.6 nm (yellow, $\mathbf{D}_3$)
$2p \to 1s$ (from the ground)	21.2 eV	58.4 nm (resonance)

The 587.6 nm D_3 line is the one by which helium was discovered in the Sun in 1868 — an l-changing ($d \to p$) dipole transition, exactly the kind RealQM captures. The dark $s \to s$ gaps ($1s^2 \to 1s2s$, the $2s$ excitations near 20 eV) are correct level spacings but not lines: they are where the outer electron lands and gets stuck, the metastability of §3.

5 What RealQM adds, and what it does not

RealQM contributes to the spectrum on two fronts. *Numbers:* the levels are computed from a non-overlapping, self-interaction-free functional whose geometric electron-avoidance captures correlation (helium -2.90 against Hartree–Fock -2.86); the line positions are RealQM's own, not borrowed, though for a difference $E_n - E_m$ the correlation partly cancels between the two levels. *Mechanism:*

radiation is a real, deterministic charge oscillation, with selection rules and metastability read as geometry rather than as matrix elements that happen to vanish.

Two things it does not do. The *structure* of the optical spectrum — one active electron in a screened core, the dipole rule — is the same as standard central-field theory; RealQM invents no new lines. And the *spin* structure is beyond it: the ortho/para (singlet–triplet) splitting is an exchange effect, and RealQM's real-valued non-overlap reproduces the spatial consequences of antisymmetry but not the spin ones. The complex, current-bearing dynamics that carries this radiation is the same one that carries magnetism (circulation) and spin: radiation is the oscillating member of that family, developed on the foundation of [2] alongside the magnetism [3] and spin [4] companions.

6 Conclusion

Atomic spectra — the birthplace of quantum mechanics and the most visible feature of an atom — are, in RealQM, real charge oscillations between real energy levels: a line is the density moving between two configurations at their difference, a dipole resonating with the field, allowed when it swings to one side and dark when it breathes symmetrically. The energies are the real theory's own, correlation-improved by the geometry of non-overlap; the mechanism is physical and deterministic — a real charge cloud in motion, not a superposition. That motion is a current, and so complex-valued in the wave function, which places radiation beside magnetism and spin in the complex time-dependent family [2, 3, 4]; what is strictly real is the levels, and the collective spin structure (ortho/para) lies beyond RealQM's non-overlap. What is gained is not a new calculation of the spectrum but a real account of it — and, for the levels themselves, numbers that geometry alone improves.

References

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