Revisiting the 1920s — with the benefit of hindsight

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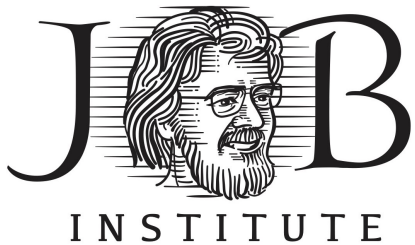

Laws of Nature Series

Towards Exact Theories of Nature

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Outline

Synopsis of textbook "Wave Mechanics" of the H atom

- First comes de Broglie's 1924 wave (+ particle) model:
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  (Often mis-represented as "electrons are waves".)
  Reproduces Bohr energy spectrum of the H atom.
  Not a dynamical theory, but a hint this might be possible.
- Next comes Schrödinger's 1926 matter-wave model.
  The solution of Schrödinger's equation for hydrogen
  reproduces Bohr energy spectrum of the H atom.
  Now there is *a* dynamics for the "de Broglie waves".
- The matter-wave interpretation leads Schrödinger to
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Not all is well, though

Schrödinger's perturbative calculations are carried out inconsistently in his matter wave model, which is non-linear and does not support his striking linear results!

Switch: Matter-wave $\longrightarrow$ Probability amplitude

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- Next comes Born's 1926 probability interpretation of Ψ, the solution of the familiar QM Schrödinger equation; more precisely: $|\Psi|^2$ as a probability density. Textbooks **do not tell** readers how this helps us to understand why atoms emit / absorb EM radiation (*with* empirical frequencies).
- Instead: One reads it requires QED to understand why there is emission / absorption of EM radiation by atoms. However, students who study QED typically only learn how to compute perturbative Feynman diagrams, and are told: Shut up and calculate!

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Shut up and calculate!

There is a better way! (A missed opportunity.)

- In the following I develop a QM model that could have been in place by the end of the 1920s, given the 1926 papers of Schrödinger and Born, the 1927 paper of de Broglie at the 5th Solvay Conference, and Pauli's 1927 spinor equation.
- First I recall Schrödinger's non-relativistic "Ψ is a matter wave" -inspired discoveries that are technically important.
- Next I revisit Schrödinger's calculations from the perspectives of Born's probability interpretation of $|\Psi|^2$, and of de Broglie's and Born's guiding-field interpretation(s) of Ψ.
- This will lead to a QM model that reproduces **all the known non-relativistic spectra** of atoms, molecules, etc., and accounts for **the emission / absorption of photons**!
- Dirac's 1928 relativistic bi-spinor equation enters next ...

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Schrödinger's hydrogen (Born-Oppenheimer approx.)

Schrödinger's equation for hydrogen reads

$$i\hbar\partial_t\Psi(t,\mathbf{s}) = \mathcal{H}^{(1)}\Psi(t,\mathbf{s}) \tag{1}$$

with

$$\mathcal{H}^{(1)} = \frac{1}{2m}\big(-i\hbar\nabla_{\mathbf{s}}\big)^2 - \frac{e^2}{|\mathbf{s}|} \tag{2}$$

"Eigen"-functions: $\Psi(t,\mathbf{s}) = e^{-iEt/\hbar}\psi(\mathbf{s}) \Longrightarrow \mathcal{H}^{(1)}\psi = E\psi$

$\mathcal{H}^{(1)}$ has ∞ many eigenvalues $E_1 < E_2 < \cdots < 0 = \inf\sigma_{\text{ess}}$.

$$E \in \left\{-\frac{me^4}{2\hbar^2}\ \frac{1}{n^2}\right\}_{n=1}^{\infty} \qquad \text{Bound States}$$

$$E \in [0,\infty) \qquad \text{Scattering States}$$

Schrödinger's Born-Oppenheimer hydrogen (cont.^{d})

Defining

$$\varrho(t,\mathbf{s}) := \Psi^*(t,\mathbf{s})\Psi(t,\mathbf{s}),$$

$$\mathbf{J}(t,\mathbf{s}) := \frac{\hbar}{m}\Im\left(\Psi^*\nabla_{\mathbf{s}}\Psi\right)(t,\mathbf{s}),$$

Schrödinger shows: the pair $(\varrho, \mathbf{J})$ satisfies the continuity equation

$$\partial_t\varrho(t,\mathbf{s}) + \nabla_{\mathbf{s}}\cdot\mathbf{J}(t,\mathbf{s}) = 0,$$

so that $\int_{\mathbb{R}^3}\varrho(t,\mathbf{s})d^3s$ is conserved if it is finite initially.
Computed with the general bound state solution, viz.

$$\Psi(t,\mathbf{s}) = \sum_{n\in\mathbb{N}} e^{-iE_nt/\hbar}\sum_{\ell=0}^{n-1}\sum_{m=-\ell}^{\ell} c_{n,\ell,m}\psi_{n,\ell,m}(\mathbf{s}),$$

his ϱ and $\mathbf{J}$ are sums of terms that oscillate harmonically with Rydberg (angular) frequencies $\omega_{n,n'} = \frac{1}{\hbar}(E_{n'} - E_n)$ for H.

Schrödinger's Born-Oppenheimer hydrogen (cont.^{d})

Schrödinger proposes that electric charge and current densities of an electron at the space point **s** at time t are given by

$$\rho_{\mathrm{el}}(t,\mathbf{s}) = -e\varrho(t,\mathbf{s}), \qquad \& \qquad \mathbf{j}_{\mathrm{el}}(t,\mathbf{s}) = -e\mathbf{J}(t,\mathbf{s}).$$

Since the charge density of an electron, ρ_{el}, integrates to $-e$, this requires the normalization

$$\int_{\mathbb{R}^3} \varrho(t,\mathbf{s})d^3s = 1.$$

Schrödinger's Born-Oppenheimer hydrogen (cont.^{d})

Using $\rho_{\rm el}(t,\mathbf{s})$ and $\mathbf{j}_{\rm el}(t,\mathbf{s})$ as source terms in the inhom. Maxwell–Lorentz equations for the EM fields of the electron,

$$-\partial_t \mathbf{E}_{\rm el}(t,\mathbf{s}) + c\nabla_{\mathbf{s}} \times \mathbf{B}_{\rm el}(t,\mathbf{s}) = 4\pi \mathbf{j}_{\rm el}(t,\mathbf{s}), \tag{3}$$

$$\nabla_{\mathbf{s}} \cdot \mathbf{E}_{\rm el}(t,\mathbf{s}) = 4\pi \rho_{\rm el}(t,\mathbf{s})\,, \tag{4}$$

coupled with the homogeneous Maxwell equations

$$\partial_t \mathbf{B}_{\rm el}(t,\mathbf{s}) + c\nabla_{\mathbf{s}} \times \mathbf{E}_{\rm el}(t,\mathbf{s}) = \mathbf{0}\,, \tag{5}$$

$$\nabla_{\mathbf{s}} \cdot \mathbf{B}_{\rm el}(t,\mathbf{s}) = 0\,, \tag{6}$$

the electric field $\mathbf{E}_{\rm el}(t,\mathbf{s})$ and the magnetic induction field $\mathbf{B}_{\rm el}(t,\mathbf{s})$ that solve this Maxwell–Lorentz system of equations are also sums of fields that oscillate with the same Rydberg hydrogen frequencies, plus an arbitrary vacuum field solution. This is a striking result (that Bohr could only postulate)!

Schrödinger's Born-Oppenheimer hydrogen (cont.^{d})

A problem: according to this calculation the hydrogen atom oscillates forever in superposition of its eigenmodes, and likewise the electromagnetic radiating goes on forever.

This is not surprising, for the feedback loop from the Maxwell–Lorentz equations for $\mathbf{E}_{\mathrm{el}}, \mathbf{B}_{\mathrm{el}}$ into Schrödinger's matter-wave equation for Ψ is missing.

Schrödinger's Born-Oppenheimer hydrogen (cont.^{d})

Schrödinger then used minimal coupling to inject $\mathbf{E}_{\rm el}, \mathbf{B}_{\rm el}$ into the matter-wave equation for Ψ. Thus he introduced the potentials $(\phi_{\rm el}(t,\mathbf{s}), \mathbf{A}_{\rm el}(t,\mathbf{s}))$, i.e. solutions to the inhomogeneous, linear partial differential equations

$$-\tfrac{1}{c}\partial_t \mathbf{A}_{\rm el}(t,\mathbf{s}) - \nabla_{\mathbf{s}}\phi_{\rm el}(t,\mathbf{s}) = \mathbf{E}_{\rm el}(t,\mathbf{s}), \tag{7}$$

$$\nabla_{\mathbf{s}} \times \mathbf{A}_{\rm el}(t,\mathbf{s}) = \mathbf{B}_{\rm el}(t,\mathbf{s}). \tag{8}$$

Note that (5) is an evolution equation for $\mathbf{A}_{\rm el}$, given $\mathbf{E}_{\rm el}$ and $\phi_{\rm el}$, while (6) is a constraint equation for $\mathbf{A}_{\rm el}$, given $\mathbf{B}_{\rm el}$. Another equation is needed, for $\phi_{\rm el}$. A compelling choice from the perspective of relativity is the *Lorenz gauge*

$$\tfrac{1}{c}\partial_t \phi_{\rm el}(t,\mathbf{s}) + \nabla_{\mathbf{s}} \cdot \mathbf{A}_{\rm el}(t,\mathbf{s}) = 0, \tag{9}$$

which is an evolution equation for $\phi_{\rm el}$.

Schrödinger's Born-Oppenheimer hydrogen (cont.^{d})

The minimal-coupling substitutions

$$E \mapsto E + e\phi_{\mathrm{el}} \qquad \& \qquad \mathbf{p} \mapsto \mathbf{p} + \tfrac{1}{c} e\mathbf{A}_{\mathrm{el}}$$

for a *test electron*, a point particle with charge $-e$ in *given* electromagnetic fields, change the Schrödinger equation to

$$\begin{aligned}(i\hbar\partial_t + e\phi_{\mathrm{el}}(t,\mathbf{s}))\,\Psi(t,\mathbf{s}) = \\ \tfrac{1}{2m}\left(-i\hbar\nabla_{\mathbf{s}} + \tfrac{e}{c}\mathbf{A}_{\mathrm{el}}(t,\mathbf{s})\right)^2\Psi(t,\mathbf{s}) - \tfrac{e^2}{|\mathbf{s}|}\Psi(t,\mathbf{s}),\end{aligned} \tag{10}$$

and the electron current vector density in the Maxwell–Lorentz equations (3)–(6) becomes

$$\mathbf{j}_{\mathrm{el}}(t,\mathbf{s}) = -e\Im\left(\Psi^*\left[\tfrac{\hbar}{m}\nabla_{\mathbf{s}} + i\tfrac{e}{mc}\mathbf{A}_{\mathrm{el}}\right]\Psi\right)(t,\mathbf{s}). \tag{11}$$

Schrödinger's Born-Oppenheimer hydrogen (cont.^{d})

By inserting "external" electromagnetic potential fields with simple periodic time dependence $\sin(\omega_{n,n'}t)$ Schrödinger showed that the solution of (10) will be resonant with a superposition of eigenmodes for E_n and $E_{n'}$.

- In 1927 Dirac then computed that if the atom is initially in an n^{th} energy level eigenstate, *in the long run* the solution Ψ of (10) will will transit either to the n'-th eigenstate or to the energy continuum! Fermi later called Dirac's formula for the transition probability per unit time

  "**Golden Rule**."

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The Schrödinger model of an *N*-electron atom (Born-Oppenheimer approximation)

We begin with an English translation of Schrödinger's own words in 1926 (**emphasis** ours):

> *"We have repeatedly called attention to the fact that the Ψ-function itself cannot and may not be interpreted directly in terms of three-dimensional space — however much the one-electron problem tends to mislead us on this point — because it is in general a function in* ***configuration space, not real space****."*
> *(Collected Papers on Wave Mechanics, p.120/1.)*

The Schrödinger model of an N-electron atom (Born-Oppenheimer approximation) (cont.^{d})

For an N-electron atom or ion with a nucleus of charge Ze fixed at the origin, with $Z \in \mathbb{N}$, now Ψ (at time t) is a function on N-particle configuration space formed with the generic positions $\vec{\boldsymbol{q}} = (\boldsymbol{q}_1, ..., \boldsymbol{q}_N) \in \mathbb{R}^{3N}$ of the N electrons. Schrödinger's N-body equation reads

$$i\hbar\partial_t \Psi(t, \vec{\boldsymbol{q}}) = \mathcal{H}^{(N)} \Psi(t, \vec{\boldsymbol{q}}) \tag{12}$$

with

$$\mathcal{H}^{(N)} = \sum_{k=1}^{N} \left(\frac{1}{2m} \big(-i\hbar\nabla_{\boldsymbol{q}_k} \big)^2 - \frac{Ze^2}{|\boldsymbol{q}_k|} \right) + \sum_{1 \le j < k \le N} \sum \frac{e^2}{|\boldsymbol{q}_j - \boldsymbol{q}_k|}. \tag{13}$$

The Schrödinger model of an N-electron atom (Born-Oppenheimer approximation) (cont.^{d})

$\mathcal{H}^{(N)}$ is essentially self-adjoint (Kato).
$\mathcal{H}^{(N)}$ has ∞ many eigenvalues $E_1 < E_2 < \cdots < \inf \sigma_{\text{ess}} \leq 0$.
Let $\boldsymbol{d}(n)$, for $n \in \mathbb{N}$ denote a finite-dimensional *degeneracy label* for the n^{th} energy eigenvalue, i.e.

$$\mathcal{H}\psi_{n,\boldsymbol{d}(n)}(\vec{\boldsymbol{q}}) = E_n \psi_{n,\boldsymbol{d}(n)}(\vec{\boldsymbol{q}}).$$

Then the general bound state solution of (12) is given by

$$\Psi(t, \vec{\boldsymbol{q}}) = \sum_{n \in \mathbb{N}} e^{-iE_n t/\hbar} \sum_{\boldsymbol{d}(n)} c_{n,\boldsymbol{d}} \psi_{n,\boldsymbol{d}(n)}(\vec{\boldsymbol{q}}). \tag{14}$$

This is all parallel to the treatment of hydrogen.

The Schrödinger model of an N-electron atom (Born-Oppenheimer approximation) (cont.^{d})

Schrödinger showed in his 4th paper of the 1926 series that

$$\varrho(t,\vec{\boldsymbol{q}}) := \Psi^*(t,\vec{\boldsymbol{q}})\Psi(t,\vec{\boldsymbol{q}})$$

and

$$\vec{\boldsymbol{J}}(t,\vec{\boldsymbol{q}}) := \tfrac{\hbar}{m}\Im\left(\Psi^*(t,\vec{\boldsymbol{q}})\nabla_{\vec{\boldsymbol{q}}}\Psi(t,\vec{\boldsymbol{q}})\right)$$

jointly satisfy the continuity equation on $\mathbb{R}\times\mathbb{R}^{3N}$,

$$\partial_t\varrho(t,\vec{\boldsymbol{q}}) + \nabla_{\vec{\boldsymbol{q}}}\cdot\vec{\boldsymbol{J}}(t,\vec{\boldsymbol{q}}) = 0; \qquad (15)$$

here, $\nabla_{\vec{\boldsymbol{q}}}\cdot$ acts in $\mathbb{R}^{3N}$, i.e. a $3N$-dim. divergence operator.

Equation (15) has the important implication that the integral $\int_{\mathbb{R}^{3N}}|\Psi|^2(t,\boldsymbol{q}_1,...,\boldsymbol{q}_N)\mathrm{d}^{3N}q$ is conserved if it is finite at $t=0$.

This is still parallel to the treatment of hydrogen.

The Schrödinger model of an N-electron atom (Born-Oppenheimer approximation) (cont.^{d})

Schrödinger proposed that Ψ's matter-wave ontology yields in physical space (and time) the many-electron charge density

$$\rho_{\mathrm{el}}(t,\mathbf{s}) = -e\sum_n \int_{\mathbb{R}^{3(N-1)}} \varrho(t,\boldsymbol{q}_1,...,\mathbf{s},...,\boldsymbol{q}_N)\mathrm{d}^{3(N-1)}q. \quad (16)$$

Similarly, he defined the many-electron current vector density

$$\mathbf{j}_{\mathrm{el}}(t,\mathbf{s}) = -e\sum_n \int_{\mathbb{R}^{3(N-1)}} \mathbf{J}_n(t,\boldsymbol{q}_1,...,\mathbf{s},...,\boldsymbol{q}_N)\mathrm{d}^{3(N-1)}q, \quad (17)$$

$$\mathbf{J}_n(t,\boldsymbol{q}_1,...,\mathbf{s},...,\boldsymbol{q}_N) := \tfrac{\hbar}{m}\Im(\Psi^*\nabla_{\mathbf{s}}\Psi)\,(t,\boldsymbol{q}_1,...,\mathbf{s},...\boldsymbol{q}_N). \quad (18)$$

In r.h.s.s(16), (17), (18), $\mathbf{s}$ is in the n-th position slot. He noted that ρ_{el} and $\mathbf{j}_{\mathrm{el}}$ jointly satisfy the continuity equation on $\mathbb{R}\times\mathbb{R}^3$.

The Schrödinger model of an N-electron atom (Born-Oppenheimer approximation) (cont.^{d})

Evaluated with the general bound state solution (14), again one finds that ϱ and $\vec{\boldsymbol{J}}$ are sums of terms that oscillate harmonically with Rydberg-Bohr-type frequencies $\omega_{n,n'} = \frac{1}{\hbar}(E_n - E_{n'})$.

Inserting ρ_{el} and $\mathbf{j}_{\mathrm{el}}$ as source terms into the inhomogeneous Maxwell–Lorentz equations (3), (4), which are coupled with the homogeneous Maxwell equations (5), (6), one obtains fields that oscillate with these Rydberg–Bohr-type frequencies. Also minimal coupling between Ψ and $(\phi_{\mathrm{el}}, \mathbf{A}_{\mathrm{el}})$ is straightforward. Thus:

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Also Dirac's **Golden Rule** calculations extend to N-electron atoms.

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Also Dirac's **Golden Rule** calculations extend to N-electron atoms.
HOWEVER: There are (at least) two conceptual inconsistencies!

Schrödinger's matter-wave model of *N*-electron atoms (de Broglie's criticism)

Here is an English translation of de Broglie's own words:

> *"We cannot recall here the successes obtained by this method ..., but we must insist on the difficulties of a conceptual type that it raises. Indeed let us consider, for simplicity, a system of N material points each possessing three degrees of freedom. The configuration space is in an essential way formed by means of the coordinates of the points, and yet Mr. Schrödinger assumes that in atomic systems material points no longer have a clearly defined position. It seems a little paradoxical to construct a configuration space with points that do not exist."* (5th *Solvay Conference, 1927)*

Schrödinger's matter-wave model for hydrogen (textbook criticism (enhanced))

A definitive assessment of the empirical viability of Schrödinger's matter-wave ontology for the *hydrogen atom* (in Born–Oppenheimer approximation) can only be obtained by non-perturbatively studying his self-consistent set of equations, nowadays known as the Schrödinger–Maxwell system.

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- The theoretical *hydrogen energy spectrum* is not reproduced $\Longrightarrow$ no Rydberg-Bohr frequencies?
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Schrödinger's matter-wave model for hydrogen (textbook criticism (enhanced)) (cont.^{d})

Ψ *does not have a physically viable matter-wave interpretation!*

Born's re-interpretation of Ψ

Born, in the 2nd paper of his 1926 series, proposed that for all practical purposes, $|\Psi|^2(t, \vec{\boldsymbol{q}})$ functions like a probability density for the first particle being at $\boldsymbol{q}_1$, the second one at $\boldsymbol{q}_2$, etc.

Born vindicated his "$|\Psi|^2$ is a probability density (FAPP)" with: "Ψ is a guiding field for the N-electron configuration!"

Born also stated that he thought the guiding equation could not be deterministic, but that Frenkel told him it could!

Born then went on to discuss scattering; he **did not** revisit Schrödinger's calculations of radiating atoms; neither did anybody else, it seems. That's what we do next!

Revisiting Schrödinger's calculations from the perspective of Born's interpretation of Ψ

For N electrons with generic positions $\boldsymbol{q}_n \in \mathbb{R}^3$, Schrödinger's many-electron 'charge density function'

$$\rho_{\mathrm{el}}(t,\mathbf{s}) = -e\sum_n \int_{\mathbb{R}^{3(N-1)}} \varrho(t,\boldsymbol{q}_1,...,\mathbf{s},...,\boldsymbol{q}_N)\mathrm{d}^{3(N-1)}q.$$

can be rewritten as

$$\rho_{\mathrm{el}}(t,\mathbf{s}) = \int_{\mathbb{R}^{3N}} \left(\sum_n - e\delta_{\boldsymbol{q}_n}(\mathbf{s})\right)|\Psi|^2(t,\vec{\boldsymbol{q}})\mathrm{d}^{3N}q,$$

and since $\varrho \equiv |\Psi|^2 \geq 0$ integrates to 1 (as Schrödinger had to stipulate), indeed this looks like the expected value of the *generic empirical charge density* $\sum_n -e\delta_{\boldsymbol{q}_n}(\mathbf{s})$ of the electrons w.r.t. a probability measure $\varrho(t,\vec{\boldsymbol{q}})\mathrm{d}^{3N}q = |\Psi|^2(t,\vec{\boldsymbol{q}})\mathrm{d}^{3N}q$.

Revisiting Schrödinger's calculations from the perspective of Born's interpretation of Ψ (cont^d)

Also Schrödinger's

$$\mathbf{j}_{\mathrm{el}}(t,\mathbf{s}) = \sum_n \int_{\mathbb{R}^{3(N-1)}} -e\tfrac{\hbar}{m}\Im(\Psi^*\nabla_{\mathbf{s}}\Psi)\,(t,\boldsymbol{q}_1,...,\mathbf{s},...\boldsymbol{q}_N)\mathrm{d}^{3(N-1)}q$$

is an expected value w.r.t. $|\Psi|^2$. We recall that the polar rep. $\Psi = |\Psi|e^{i\Phi}$ yields $\Im(\Psi^*\nabla\Psi) = |\Psi|^2\nabla\Phi$. Thus, for each n,

$$\Im\big(\Psi^*(t,\vec{\boldsymbol{q}})\nabla_{\boldsymbol{q}_n}\Psi(t,\vec{\boldsymbol{q}})\big) = |\Psi|^2(t,\vec{\boldsymbol{q}})\nabla_{\boldsymbol{q}_n}\Phi(t,\vec{\boldsymbol{q}}),$$

and so

$$\mathbf{j}_{\mathrm{el}}(t,\mathbf{s}) = \int_{\mathbb{R}^{3N}}\Big(\sum_n - e\tfrac{\hbar}{m}\mathcal{I}_n\big(\nabla_{\boldsymbol{q}_n}\Phi(t,\vec{\boldsymbol{q}})\big)\delta_{\boldsymbol{q}_n}(\mathbf{s})\Big)|\Psi|^2(t,\vec{\boldsymbol{q}})\mathrm{d}^{3N}q.$$

We note that Φ *is generally not a function of* $|\Psi|^2$.

de Broglie's contribution: the guiding equation

We summarize:

ρ_{el} can be expressed as the expected value w.r.t. $|\Psi|^2$ of the electrons' *generic electrical charge density*

$$\sum_n -e\delta_{\boldsymbol{q}_n}(\mathbf{s}).$$

$\mathbf{j}_{\mathrm{el}}$ can be expressed as expected value w.r.t. $|\Psi|^2$ of the electrons' *generic electrical current vector density*

$$\sum_n -e\frac{\hbar}{m}\mathcal{I}_n\big(\nabla_{\boldsymbol{q}_n}\Phi(t,\vec{\boldsymbol{q}})\big)\delta_{\boldsymbol{q}_n}(\mathbf{s}),$$

Enter de Broglie's insight: $\frac{\hbar}{m}\nabla_{\boldsymbol{q}_n}\Phi(t,\vec{\boldsymbol{q}})$ must be interpreted as the n-th component $\boldsymbol{v}_n$ of a *generic velocity field* $\vec{\boldsymbol{v}}$ on configuration space $\mathbb{R}^{3N}$. Thus, if $\vec{\boldsymbol{q}}(t)$ is the actual N-electron configuration, then it evolves according to the deterministic ODE

$$\boxed{\frac{d}{dt}\vec{\boldsymbol{q}}(t) = \vec{\boldsymbol{v}}\big(t,\vec{\boldsymbol{q}}(t)\big)}\,.$$

(Born did not appreciate this!)

Average sources produce average fields

Schrödinger's calculations from a de Broglie–Born perspective:

- If "source" means "expected value of generic source," then "field" in the symbolic Maxwell–Lorentz equations

$$D\,\textbf{field} \;=\; \textbf{source}$$

should be interpreted as "expected value of generic field."

- Moreover, "D (*expected value of generic field*)" should be identical with "*expected value of* $\widetilde{D}$ (*generic field*)."
- Those generic fields must be 3-dim. vector fields $\mathbf{E}^\sharp$ and $\mathbf{B}^\sharp$ on spacetime $(t, \mathbf{s})$ that depend on the generic $\vec{q}$.
- The differential operator $\widetilde{D}$ acts on $(t, \mathbf{s})$ and $\vec{q}$ variables, while D acts only on the time and space variables $(t, \mathbf{s})$.

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Generic Maxwell–Lorentz field equations

There are two inhomogeneous equations for the $\sharp$ fields,

$$\partial_t \mathbf{E}^\sharp + \big(\sum_k \boldsymbol{v}_k \cdot \nabla_{\boldsymbol{q}_k}\big)\mathbf{E}^\sharp - c\nabla_{\mathbf{s}} \times \mathbf{B}^\sharp = 4\pi e \sum_n \mathcal{I}_n \boldsymbol{v}_n \delta_{\boldsymbol{q}_n}(\mathbf{s}),$$

$$\nabla_{\mathbf{s}} \cdot \mathbf{E}^\sharp = 4\pi e\big(Z\delta_{\mathbf{0}}(\mathbf{s}) - \sum_n \delta_{\boldsymbol{q}_n}(\mathbf{s})\big),$$

and two homogeneous equations,

$$\partial_t \mathbf{B}^\sharp + \big(\sum_k \boldsymbol{v}_k \cdot \nabla_{\boldsymbol{q}_k}\big)\mathbf{B}^\sharp + c\nabla_{\mathbf{s}} \times \mathbf{E}^\sharp = \mathbf{0}\,,$$

$$\nabla_{\mathbf{s}} \cdot \mathbf{B}^\sharp = 0\,,$$

where, for brevity, we have suppressed the arguments from $\mathbf{E}^\sharp(t, \mathbf{s}; \vec{\boldsymbol{q}})$ and $\mathbf{B}^\sharp(t, \mathbf{s}; \vec{\boldsymbol{q}})$, and we wrote $\boldsymbol{v}_n$ for $\boldsymbol{v}_n(t, \vec{\boldsymbol{q}})$.

Generic Maxwell–Lorentz field equations (cont.^{d})

Substituting the *actual electron positions at time* t, i.e. $\vec{\boldsymbol{q}}(t)$, for the generic $\vec{\boldsymbol{q}}$ in the $\sharp$-fields, these become electromagnetic fields of $\mathbf{s}$ and t,

$$\mathbf{E}^{\sharp}(t,\mathbf{s};\vec{\boldsymbol{q}}(t)) = \mathbf{E}(t,\mathbf{s}) \quad \text{and} \quad \mathbf{B}^{\sharp}(t,\mathbf{s};\vec{\boldsymbol{q}}(t)) = \mathbf{B}(t,\mathbf{s}),$$

satisfying the Maxwell–Lorentz field equations

$$\partial_t \mathbf{E}(t,\mathbf{s}) - c\nabla_{\mathbf{s}} \times \mathbf{B}(t,\mathbf{s}) = 4\pi e \sum_n \mathcal{I}_n \dot{\boldsymbol{q}}_n(t)\delta_{\boldsymbol{q}_n(t)}(\mathbf{s}),$$
$$\nabla_{\mathbf{s}} \cdot \mathbf{E}(t,\mathbf{s}) = 4\pi e\big(Z\delta_{\mathbf{0}}(\mathbf{s}) - \sum_n \delta_{\boldsymbol{q}_n(t)}(\mathbf{s})\big),$$

$$\partial_t \mathbf{B}(t,\mathbf{s}) + c\nabla_{\mathbf{s}} \times \mathbf{E}(t,\mathbf{s}) = \mathbf{0}\,,$$
$$\nabla_{\mathbf{s}} \cdot \mathbf{B}(t,\mathbf{s}) = 0\,.$$

Generic Maxwell–Lorentz field equations (cont.^{d})

Averaging w.r.t. $|\Psi|^2 = \varrho$ turns the generic ML equations into

$$\left(-\partial_t \langle \mathbf{E}^\sharp \rangle + c\nabla_{\mathbf{s}} \times \langle \mathbf{B}^\sharp \rangle\right)(t,\mathbf{s}) = 4\pi\, \langle \mathbf{j}_{\mathrm{el}}^{\mathrm{emp}} \rangle (t,\mathbf{s}), \tag{19}$$

$$\nabla_{\mathbf{s}} \cdot \langle \mathbf{E}^\sharp \rangle (t,\mathbf{s}) = 4\pi \left(\langle \rho_{\mathrm{el}}^{\mathrm{emp}} \rangle (t,\mathbf{s}) + Ze\delta_{\mathbf{0}}(\mathbf{s}) \right), \tag{20}$$

$$\left(\partial_t \langle \mathbf{B}^\sharp \rangle + c\nabla_{\mathbf{s}} \times \langle \mathbf{E}^\sharp \rangle\right)(t,\mathbf{s}) = \mathbf{0}\,, \tag{21}$$

$$\nabla_{\mathbf{s}} \cdot \langle \mathbf{B}^\sharp \rangle (t,\mathbf{s}) = 0\,. \tag{22}$$

Thus the ϱ-averaged $\sharp$-field equations for the generic empirical sources are precisely the four Maxwell–Lorentz field equations (3)–(6) for the electrons' electromagnetic field, with Schrödinger's expression (17) at r.h.s. (3) and his (16) at r.h.s.(4), except that here we have also included the charge density of the point nucleus at r.h.s.(20).

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- For few-body systems, dramatic deviations from the rules of relativity theory may occur, as in Bell-type experiments.
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Feedback of electrostatic Maxwell ♯-fields to Ψ

Replacing point charges by tiny charged balls of radius a, and suppressing t as argument in the ♯ fields, we now recall a well-known result from the classical theory of electrostatics:

Assume that pairwise $|\boldsymbol{q}_j - \boldsymbol{q}_k| > 2a$, and that all $|\boldsymbol{q}_k| > 2a$, so that no two charge balls overlap. Then the electrostatic field energy of such a generic $N+1$ charge configuration, with the field being the sum of the Coulomb fields of all charged balls, is

$$\frac{1}{8\pi}\int_{\mathbb{R}^3}\left|\mathbf{E}^\sharp(\mathbf{s};\vec{\boldsymbol{q}})\right|^2 \mathrm{d}^3 s = E_{\text{self}} - \sum_{n=1}^{N}\frac{Ze^2}{|\boldsymbol{q}_n|} + \sum_{1\le j<k\le N}\sum\frac{e^2}{|\boldsymbol{q}_j - \boldsymbol{q}_k|},$$

and except for the configuration-independent "self-field" energy $E_{\text{self}} = \frac{3}{5}\frac{e^2}{a}\left(Z^2+N\right)$ this is precisely the interaction term in Schrödinger's equation (12) with hamiltonian $\mathcal{H}^{(N)}$ given by (13).

Feedback of generic Maxwell ♯-fields to Ψ

The formulas obtained for the electrostatic special case suggest that at least part of the back coupling of the electromagnetic fields into the Schrödinger equation is obtained from the field energy of the ♯ fields sourced by generic point charge densities and current densities, given by

$$E^{\sharp}(t,\vec{\boldsymbol{q}}) := \frac{1}{8\pi}\int_{\mathbb{R}^3}\left(\left|\mathbf{E}^{\sharp}(t,\mathbf{s};\vec{\boldsymbol{q}})\right|^2+\left|\mathbf{B}^{\sharp}(t,\mathbf{s};\vec{\boldsymbol{q}})\right|^2\right)\mathrm{d}^3s. \qquad (23)$$

This includes the "minimally coupled external electric potential."

Feedback of generic Maxwell ♯-fields to Ψ

This now suggests that the field momentum of the electromagnetic ♯ fields,

$$\boldsymbol{P}^{\sharp}(t,\vec{\boldsymbol{q}}) := \frac{1}{4\pi c}\int_{\mathbb{R}^3} \mathbf{E}^{\sharp}(t,\mathbf{s};\vec{\boldsymbol{q}}) \times \mathbf{B}^{\sharp}(t,\mathbf{s};\vec{\boldsymbol{q}})\mathrm{d}^3 s, \qquad (24)$$

injected into the n-th component of $T_{\vec{\boldsymbol{q}}}\mathbb{R}^{3N}$, may take the place of a "minimally coupled external magnetic vector potential," but this overcounts the contributions to the n^{th} canonical momentum. The linearity of the ♯ field equations comes to the rescue.

Decomposition of generic Maxwell ♯-fields

We decompose

$$\mathbf{E}^{\sharp}(t,\mathbf{s};\vec{\boldsymbol{q}}) = \mathbf{E}^{\mathrm{ext}}(t,\mathbf{s}) + \sum_{n=1}^{N} \mathbf{E}^{\sharp}_{n}(t,\mathbf{s};\vec{\boldsymbol{q}})$$

$$\mathbf{B}^{\sharp}(t,\mathbf{s};\vec{\boldsymbol{q}}) = \mathbf{B}^{\mathrm{ext}}(t,\mathbf{s}) + \sum_{n=1}^{N} \mathbf{B}^{\sharp}_{n}(t,\mathbf{s};\vec{\boldsymbol{q}}).$$

Here, $\mathbf{E}^{\mathrm{ext}}(t,\mathbf{s})$ and $\mathbf{B}^{\mathrm{ext}}(t,\mathbf{s})$ are classical electromagnetic Maxwell–Lorentz fields sourced by the charge density $Ze\delta^{(a)}_{\mathbf{0}}$ of the nucleus and possibly other compactly supported external sources $\rho^{\mathrm{ext}}_{\mathrm{lab}}(t,\mathbf{s})$ and $\mathbf{j}^{\mathrm{ext}}_{\mathrm{lab}}(t,\mathbf{s})$ located far away from the atom, obeying the continuity equation for external charge conservation.

Decomposition of generic Maxwell ♯-fields

The external fields satisfy the Maxwell–Lorentz field equations

$$-\partial_t \mathbf{E}^{\text{ext}}(t,\mathbf{s}) + c\nabla_{\mathbf{s}} \times \mathbf{B}^{\text{ext}}(t,\mathbf{s}) = 4\pi \mathbf{j}^{\text{ext}}_{\text{lab}}(t,\mathbf{s}), \tag{25}$$

$$\nabla_{\mathbf{s}} \cdot \mathbf{E}^{\text{ext}}(t,\mathbf{s}) = 4\pi \left(Ze\delta^{(a)}_{\mathbf{0}}(\mathbf{s}) + \rho^{\text{ext}}_{\text{lab}}(t,\mathbf{s}) \right), \tag{26}$$

$$\partial_t \mathbf{B}^{\text{ext}}(t,\mathbf{s}) + c\nabla_{\mathbf{s}} \times \mathbf{E}^{\text{ext}}(t,\mathbf{s}) = \mathbf{0}, \tag{27}$$

$$\nabla_{\mathbf{s}} \cdot \mathbf{B}^{\text{ext}}(t,\mathbf{s}) = 0. \tag{28}$$

Decomposition of generic Maxwell ♯-fields

Again suppressing, for brevity, the arguments from the n-th velocity field component $\boldsymbol{v}_n(t,\vec{\boldsymbol{q}})$, to be defined below, and from $\mathbf{E}^{\sharp}(t,\mathbf{s};\vec{\boldsymbol{q}})$ and $\mathbf{B}^{\sharp}(t,\mathbf{s};\vec{\boldsymbol{q}})$, the n-th ♯ fields satisfy the two inhomogeneous equations

$$-\partial_t \mathbf{E}^{\sharp}_n - \big(\sum_k \boldsymbol{v}_k\cdot\nabla_{\boldsymbol{q}_k}\big)\mathbf{E}^{\sharp}_n + c\nabla_{\mathbf{s}}\times\mathbf{B}^{\sharp}_n = 4\pi\mathcal{I}_n\big(-e\boldsymbol{v}_n\delta^{(a)}_{\boldsymbol{q}_n}(\mathbf{s})\big), \quad (29)$$

$$\nabla_{\mathbf{s}}\cdot\mathbf{E}^{\sharp}_n = 4\pi\big(-e\delta^{(a)}_{\boldsymbol{q}_n}(\mathbf{s})\big), \quad (30)$$

and the two homogeneous equations,

$$\partial_t \mathbf{B}^{\sharp}_n + \big(\sum_k \boldsymbol{v}_k\cdot\nabla_{\boldsymbol{q}_k}\big)\mathbf{B}^{\sharp}_n + c\nabla_{\mathbf{s}}\times\mathbf{E}^{\sharp}_n = \mathbf{0}\,, \quad (31)$$

$$\nabla_{\mathbf{s}}\cdot\mathbf{B}^{\sharp}_n = 0\,. \quad (32)$$

Feedback of generic Maxwell ♯-fields to Ψ

We now define

$$\boldsymbol{P}_n^\sharp(t,\vec{\boldsymbol{q}}) := \mathcal{I}_n^{-1}\frac{1}{4\pi c}\int_{\mathbb{R}^3}\left(\mathbf{E}_n^\sharp\times\mathbf{B}^\sharp\right)(t,\mathbf{s};\vec{\boldsymbol{q}})\mathrm{d}^3s$$

and propose

$$\boxed{\left(i\hbar\partial_t - E^\sharp(t,\vec{\boldsymbol{q}})\right)\Psi(t,\vec{\boldsymbol{q}}) = \sum_{n=1}^{N}\frac{1}{2m}\left(-i\hbar\nabla_{\boldsymbol{q}_n} - \boldsymbol{P}_n^\sharp(t,\vec{\boldsymbol{q}})\right)^2\Psi(t,\vec{\boldsymbol{q}})}$$

as our Schrödinger wave equation for Ψ, coupled to the ♯ fields. Note that $E^\sharp$ and the $\boldsymbol{P}_n^\sharp$ occupy the slots of the external electromagnetic potentials in minimal coupling procedure.

Conservation of L^2 norm of Ψ

It follows right away that

$$\varrho(t,\vec{\boldsymbol{q}}) := \Psi^*(t,\vec{\boldsymbol{q}})\Psi(t,\vec{\boldsymbol{q}}),$$

and $\vec{\boldsymbol{J}}$, having n-th component

$$\mathbf{J}_n(t,\vec{\boldsymbol{q}}) := \Im\left(\Psi^*(t,\vec{\boldsymbol{q}})\tfrac{1}{m}\left(\hbar\nabla_{\boldsymbol{q}_n} - i\boldsymbol{P}_n^\sharp(t,\vec{\boldsymbol{q}})\right)\Psi(t,\vec{\boldsymbol{q}})\right),$$

jointly satisfy the continuity equation (15), viz.

$$\boxed{\partial_t\varrho(t,\vec{\boldsymbol{q}}) + \nabla_{\vec{\boldsymbol{q}}}\cdot\vec{\boldsymbol{J}}(t,\vec{\boldsymbol{q}}) = 0}.$$

As a consequence, the $L^2(\mathbb{R}^{3N})$ norm of $\Psi(t,\vec{\boldsymbol{q}})$ is conserved.

Velocity field generated by Ψ / Guiding law

Using the polar decomposition $\Psi = |\Psi| e^{i\Phi}$, we have the familiar

$$\Im\left(\Psi^*(t,\vec{\boldsymbol{q}})\nabla_{\vec{\boldsymbol{q}}}\Psi(t,\vec{\boldsymbol{q}})\right) = |\Psi|^2(t,\vec{\boldsymbol{q}})\nabla_{\vec{\boldsymbol{q}}}\Phi(t,\vec{\boldsymbol{q}}),$$

and therefore $\vec{\boldsymbol{J}}(t,\vec{\boldsymbol{q}}) = \varrho(t,\vec{\boldsymbol{q}})\vec{\boldsymbol{v}}(t,\vec{\boldsymbol{q}})$ with $\vec{\boldsymbol{v}}$ given by

$$\forall\, n:\ \ \boldsymbol{v}_n(t,\vec{\boldsymbol{q}}) = \frac{1}{m}\left(\hbar\nabla_{\boldsymbol{q}_n}\Phi(t,\vec{\boldsymbol{q}}) - \boldsymbol{P}_n^{\sharp}(t,\vec{\boldsymbol{q}})\right), \qquad (33)$$

which is to be used in the ♯-field equations.
The actual positions of the electrons, $\boldsymbol{q}_n(t)$, are postulated to evolve in time according to the pertinent de Broglie–Bohm-type guiding equation

$$\boxed{\forall\, n:\quad \frac{\mathrm{d}\boldsymbol{q}_n(t)}{\mathrm{d}t} = \frac{1}{m}\left(\hbar\nabla_{\boldsymbol{q}_n}\Phi(t,\vec{\boldsymbol{q}}) - \boldsymbol{P}_n^{\sharp}(t,\vec{\boldsymbol{q}})\right)\Big|_{\vec{\boldsymbol{q}}=\vec{\boldsymbol{q}}(t)}}. \qquad (34)$$

Feedback of generic Maxwell$^\sharp$ fields to Ψ with spin

To include electron spin, replace the N-electron Schrödinger-type equation with the N-electron Pauli-type equation

$$\left(i\hbar\partial_t - E^\sharp(t,\vec{\boldsymbol{q}})\right)\Psi(t,\vec{\boldsymbol{q}}) = \sum_{n=1}^{N}\frac{1}{2m}\left(\boldsymbol{\sigma}_n\cdot\left(-i\hbar\nabla_{\boldsymbol{q}_n} - \boldsymbol{P}_n^\sharp(t,\vec{\boldsymbol{q}})\right)\right)^2\Psi(t,\vec{\boldsymbol{q}}),$$

with $\Psi(t,\vec{\boldsymbol{q}})$ an N-body Pauli spinor wave function that is antisymmetric under the permutation group S_N.
The spinor prob.-density $\varrho = \Psi^\dagger\Psi$ (= sum of $|\Psi_k|^2$ over all 2^N components), and the prob. current density has n^{th} component

$$\mathbf{J}_n(t,\vec{\boldsymbol{q}}) = \Im\left(\Psi^\dagger\frac{1}{m}\left(\hbar\nabla_{\boldsymbol{q}_n} - i\boldsymbol{P}_n^\sharp\right)\Psi\right)(t,\vec{\boldsymbol{q}}) + \frac{1}{2m}\hbar\nabla_{\boldsymbol{q}_n}\times\left(\Psi^\dagger\boldsymbol{\sigma}_n\Psi\right)(t,\vec{\boldsymbol{q}});$$

the curl term is optional, yet suggested by Dirac's equation.
The velocity field is again defined by $\vec{\boldsymbol{J}} = \varrho\vec{\boldsymbol{v}}$.

Systems with many nuclei (Born-Oppenheimer approx.)

The many-electron Pauli equation governs the evolution of the N-electron wave function with spin unchanged in appearance, yet the $\boldsymbol{P}_n^\sharp$ and $E^\sharp$ are computed from solutions to the $\sharp$-field equations in which the source term includes K nuclei, i.e.

$$\nabla_{\mathbf{s}} \cdot \mathbf{E}^\sharp = 4\pi e\Big(\sum_{k=1}^{K} Z_k \delta^{(a)}_{\boldsymbol{q}_k^+}(\mathbf{s}) - \sum_{n=1}^{N} \delta^{(a)}_{\boldsymbol{q}_n}(\mathbf{s})\Big), \tag{35}$$

where the positions of the nuclei are distinguished from those of the electrons by the superscript $^+$.

Systems with many nuclei (Born-Oppenheimer approx.)

Provided no two charged balls of radius a overlap, the energy of the pertinent electrostatic $\sharp$ field solution now reads

$$\frac{1}{8\pi}\int_{\mathbb{R}^3}\left|\mathbf{E}^{\sharp}(\mathbf{s};\vec{\boldsymbol{q}}\,|\,\vec{\boldsymbol{q}}^{+})\right|^2\mathrm{d}^3s = E_{\text{self}} + \sum\sum_{1\le j<k\le K}\frac{Z_jZ_ke^2}{|\boldsymbol{q}_j^+-\boldsymbol{q}_k^+|} - \sum_{k=1}^{K}\sum_{n=1}^{N}\frac{Z_ke^2}{|\boldsymbol{q}_n-\boldsymbol{q}_k^+|} + \sum\sum_{1\le j<k\le N}\frac{e^2}{|\boldsymbol{q}_j-\boldsymbol{q}_k|},$$

with the constant self-energy $E_{\text{self}} = \frac{3}{5}\frac{e^2}{a}\left(N+\sum_{k=1}^{K}Z_k^2\right)$; for smaller distances the Coulomb interactions are smoothed out. The nuclei positions $\boldsymbol{q}_k^+$ are "classical parameters"; yet this 1927 Born-Oppenheimer approximation can easily be relaxed. Laboratory-generated static external fields can be included.

Emission / Absorption of Radiation (just Hydrogen)

We need to solve the ♯-field equations (as initial value problem). After separating off the static Coulomb field from the radiation fields — incoming vacuum fields plus outgoing sourced fields,

$$\mathbf{B}^{\sharp,s}_{\mathrm{rad}}(t,\mathbf{s};\boldsymbol{q}) = \nabla_{\mathbf{s}} \times \mathbf{A}^{\sharp,s}_{\mathrm{rad}}(t,\mathbf{s};\boldsymbol{q})\ ,$$
$$\mathbf{E}^{\sharp,s}_{\mathrm{rad}}(t,\mathbf{s},\boldsymbol{q}) = -\tfrac{1}{c}\tfrac{\partial}{\partial t}\mathbf{A}^{\sharp,s}_{\mathrm{rad}}(t,\mathbf{s};\boldsymbol{q}) - \tfrac{1}{c}\big(\boldsymbol{v}(t,\boldsymbol{q})\cdot\nabla_{\boldsymbol{q}}\big)\mathbf{A}^{\sharp,s}_{\mathrm{rad}}(t,\mathbf{s};\boldsymbol{q}),$$

the latter can be solved for by the method of characteristics:

$$\mathbf{A}^{\sharp,s}_{\mathrm{rad}}(t,\mathbf{s};\boldsymbol{q}) = -2\tfrac{e}{c}\left.\frac{\big(\frac{d}{d\tau}\boldsymbol{Q}_{\boldsymbol{q}}(\tau)\big)^{\perp}_{\boldsymbol{n}_{\tau,\mathbf{s}}}}{|\boldsymbol{Q}_q(\tau)-\mathbf{s}|}\right|_{\tau=t^{\mathrm{ret}}(t,\mathbf{s};\boldsymbol{q})} \tag{36}$$
$$+\,2\tfrac{e}{c}\int_0^t \left(\big(\tfrac{d}{d\tau}\boldsymbol{Q}_{\boldsymbol{q}}(\tau)\big)^{\perp}_{\boldsymbol{n}_{\tau,\mathbf{s}}} - 2\big(\tfrac{d}{d\tau}\boldsymbol{Q}_{\boldsymbol{q}}(\tau)\big)^{\parallel}_{\boldsymbol{n}_{\tau,\mathbf{s}}}\right)\frac{c(t-\tau)}{|\boldsymbol{Q}_q(\tau)-\mathbf{s}|}\mathbf{1}_{\{\tau>t^{\mathrm{ret}}(t,\mathbf{s};\boldsymbol{q})\}}\,d\tau.$$

This is for $a = 0$; to obtain the ♯-field vector potential for the ♯-fields with $a > 0$, convolute (36) w.r.t. its $\boldsymbol{q}$ variable with the normalized characteristic function of the ball of radius a

Emission / Absorption of Radiation (Hydrogen) (cont.^{d})

In the solution formula for $\mathbf{A}^{\sharp,s}_{\text{rad}}(t,\mathbf{s};\boldsymbol{q})$, the "retarded (instant of) time" $t^{\text{ret}}(t,\mathbf{s};\boldsymbol{q})$ is defined implicitly as solution of

$$c(t-t^{\text{ret}}) = |\mathbf{s} - \boldsymbol{Q}_{\boldsymbol{q}}(t^{\text{ret}})|,$$

where we have also set $\boldsymbol{Q}_q(t^{\text{ret}}) = \boldsymbol{Q}_q(0)$ if $t^{\text{ret}} < 0$.

Emission / Absorption of Radiation (Hydrogen) (cont.^{d})

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where we also set $\boldsymbol{Q}_q(t^{\mathrm{ret}}) = \boldsymbol{Q}_q(0)$ if $t^{\mathrm{ret}} < 0$.

Here, $\tau \mapsto \boldsymbol{Q}_{\boldsymbol{q}}(\tau)\big)$ solves the de Broglie–Bohm guiding equation

$$\boxed{\frac{d}{d\tau}\boldsymbol{Q}_{\boldsymbol{q}}(\tau) = \boldsymbol{v}(\tau, \boldsymbol{Q}_{\boldsymbol{q}}(\tau))} \tag{37}$$

as *final value problem*, with $\boldsymbol{Q}_{\boldsymbol{q}}(t) = \boldsymbol{q}$.

REVELATION: characteristics are de Broglie–Bohm motions!

Emission / Absorption of Radiation (Hydrogen) (cont.^{d})

Initial value problem:

Hydrogen $\Psi(0, \boldsymbol{q})$ is a bound state (say: a first excited state);

Radiation $\sharp$-field is incoming Gaussian beam pulse with a Rydberg frequency $\omega_{2,1}$ of energy $= O(\epsilon)$;

Established to first-order in ϵ:

After passing of the pulse the atom will be in superposition of $n = 1$ and $n = 2$ state (selection rule!);

There will be a spherical outgoing EM-field wave with a Rydberg frequency $\omega_{2,1}$ (selection rule!).

Expected: Atom will settle down in ground state. (Golden Rule?)
(Not yet shown rigorously.)

EM Fields vs. Photons

The emitted expected radiation ♯-fields form an essentially spherical shell of radius $\approx ct$.

Clearly this is not what seems to happen in experiments:

an atom that transits from an excited state to its ground state does so under the emission of photons, which get registered in localized photon detectors.

Spherical EM radiation cannot account for such an event.

A single Photon

However, the following notationally trivial, but conceptually radical change of perspective brings the photon into the model!
Contemplate that the variable **s** in the ♯ fields and their ♯-field equations does not represent a generic point in physical space, but instead represents the generic position of a photon!
Replace the space point by the position variable of a photon,

$$\mathbf{s} \longrightarrow \boldsymbol{q}_{\mathrm{ph}}$$

and introduce a suffix at the electron positions,

$$\boldsymbol{q} \longrightarrow \boldsymbol{q}_{\mathrm{el}}$$

and for N electrons,

$$\vec{\boldsymbol{q}} \longrightarrow \vec{\boldsymbol{q}}_{\mathrm{el}}$$

to distinguish the two types of position $\boldsymbol{q}$-variables.

A single Photon (cont.^{d})

Now following Heinrich Weber (1902), set

$$\mathbf{E}^\sharp(t, \boldsymbol{q}_{\rm ph}; \vec{\boldsymbol{q}}_{\rm el}) + i\, \mathbf{B}^\sharp(t, \boldsymbol{q}_{\rm ph}; \vec{\boldsymbol{q}}_{\rm el}) =: e\hbar \boldsymbol{\Psi}(t, \boldsymbol{q}_{\rm ph}; \vec{\boldsymbol{q}}_{\rm el}).$$

The $\sharp$-field equations then rewrite as

$$\left[i\hbar\partial_t + c\hbar \left(\nabla_{\boldsymbol{q}_{\rm ph}} \times \right) + i\hbar \left(\vec{\boldsymbol{v}}(t, \vec{\boldsymbol{q}}_{\rm el}) \cdot \nabla_{\vec{\boldsymbol{q}}_{\rm el}} \right) \right] \boldsymbol{\Psi}(t, \boldsymbol{q}_{\rm ph}; \vec{\boldsymbol{q}}_{\rm el})$$
$$= 4\pi \vec{\boldsymbol{v}}(t, \vec{\boldsymbol{q}}_{\rm el}) \cdot \delta^{(a)}_{\vec{\boldsymbol{q}}_{\rm el}}(\boldsymbol{q}_{\rm ph}),$$
$$\hbar \nabla_{\boldsymbol{q}_{\rm ph}} \cdot \boldsymbol{\Psi}(t, \boldsymbol{q}_{\rm ph}; \vec{\boldsymbol{q}}_{\rm el}) = 4\pi \Big(\delta^{(a)}_{\boldsymbol{0}}(\boldsymbol{q}_{\rm ph}) - \sum_n \delta^{(a)}_{\boldsymbol{q}_{{\rm el},n}}(\boldsymbol{q}_{\rm ph}) \Big).$$

Multiplying by ϱ and recalling that $\varrho \vec{\boldsymbol{v}} = \vec{\boldsymbol{J}}$, the bilinear feedback from the Ψ equation into the $\boldsymbol{\Psi}$ equations puts the coupled system of equations on a more equal footing.

A single Photon (cont.^{d})

But when $\boldsymbol{\Psi}(t, \boldsymbol{q}_{\mathrm{ph}}; \vec{\boldsymbol{q}}_{\mathrm{el}})$ lives on the joint configuration space for electrons and photon, it is very tempting to let oneself be inspired by the speculations of de Broglie, Born, and Bohm, and to think of $\boldsymbol{\Psi}(t, \boldsymbol{q}_{\mathrm{ph}}; \vec{\boldsymbol{q}}_{\mathrm{el}})$ as a guiding field for the photon.

Thus we need the guiding equation for the actual position of the photon in physical space. It is suggestive in this (semi-relativistic) setting to postulate (tentatively) that the photon position at time t, say $\boldsymbol{q}_{\mathrm{ph}}(t)$, moves as per the guiding equation

$$\frac{\mathrm{d}\boldsymbol{q}_{\mathrm{ph}}(t)}{\mathrm{d}t} = c \frac{\Im\left(\boldsymbol{\Psi}^*(t, \boldsymbol{q}_{\mathrm{ph}}; \vec{\boldsymbol{q}}_{\mathrm{el}}(t)) \times \boldsymbol{\Psi}(t, \boldsymbol{q}_{\mathrm{ph}}; \vec{\boldsymbol{q}}_{\mathrm{el}}(t))\right)}{\boldsymbol{\Psi}^*(t, \boldsymbol{q}_{\mathrm{ph}}; \vec{\boldsymbol{q}}_{\mathrm{el}}(t)) \cdot \boldsymbol{\Psi}(t, \boldsymbol{q}_{\mathrm{ph}}; \vec{\boldsymbol{q}}_{\mathrm{el}}(t))} \Bigg|_{\boldsymbol{q}_{\mathrm{ph}} = \boldsymbol{q}_{\mathrm{ph}}(t)}.$$

A single Photon (cont.^{d})

Remark: *Einstein was pondering a guiding field for photons (his "quanta of light") on physical spacetime, obeying a relativistic field equation. We noted already that the evaluation of the ♯ fields with the actual electron positions* $\vec{\boldsymbol{q}}_{\mathrm{el}}(t)$ *in place of the generic* $\vec{\boldsymbol{q}}_{\mathrm{el}}$ *turns the ♯ fields into solutions of the classical Maxwell–Lorentz field equations for point charges, except that the motions are not generated by a classical law.*
In this sense the guiding equation for the photon would seem to come as close as it can get to realizing Einstein's surmise that the classical electromagnetic field guides the photons.

Many Photons

There are a number of requirements that a generalization of our model to a system of equations for a hydrogen atom in the presence of many photons needs to satisfy. First of all, since photons are spin 1 bosons, their quantum-mechanical many-body wave function $\boldsymbol{\Psi}$ has to be permutation-symmetric. The generalized L-photon ♯-field $\boldsymbol{\Psi}(t, \vec{\boldsymbol{q}}_{\rm ph}; \vec{\boldsymbol{q}}_{\rm el})$ thus takes values in the closure of the L-fold symmetrized tensor products of single-photon $\boldsymbol{\Psi}(t, \boldsymbol{q}^{\ell}_{\rm ph}; \vec{\boldsymbol{q}}_{\rm el})$ over $\ell = 1, ..., L$. Second, the stationary states must produce the same hydrogen spectrum as when only a single photon was present.
Third, ... more (but let's make sure we get the first two right!)

Many Photons (cont.[d])

It is then straightforward to verify that our single-photon ♯-field equations (in Weber notation) are the single-photon special case of the following equations for the L-photon sector,

$$\left(i\hbar\partial_t + c\hbar\sum_\ell \nabla_{\boldsymbol{q}^\ell_{\rm ph}} \times_\ell + i\hbar\vec{\boldsymbol{v}}(t,\vec{\boldsymbol{q}}_{\rm el})\cdot\nabla_{\vec{\boldsymbol{q}}_{\rm el}}\right)\boldsymbol{\Psi}^L(t,\vec{\boldsymbol{q}}_{\rm ph};\vec{\boldsymbol{q}}_{\rm el})$$

$$= 4\pi\tfrac{1}{\sqrt{L}}\sum_\ell \boldsymbol{\Psi}^{L-1}(t,\vec{\boldsymbol{q}}^{\hat{\ell}}_{\rm ph};\vec{\boldsymbol{q}}_{\rm el})\otimes_\ell \vec{\boldsymbol{v}}(t,\vec{\boldsymbol{q}}_{\rm el})\cdot\delta^{(a)}_{\vec{\boldsymbol{q}}_{\rm el}}(\boldsymbol{q}^\ell_{\rm ph}),$$

$$\hbar\nabla_{\vec{\boldsymbol{q}}_{\rm ph}}\cdot\boldsymbol{\Psi}^L(t,\vec{\boldsymbol{q}}_{\rm ph};\vec{\boldsymbol{q}}_{\rm el}) = 4\pi\tfrac{1}{\sqrt{L}}\sum_\ell \boldsymbol{\Psi}^{L-1}(t,\vec{\boldsymbol{q}}^{\hat{\ell}}_{\rm ph};\vec{\boldsymbol{q}}_{\rm el})\left(\delta^{(a)}_{\boldsymbol{0}}(\boldsymbol{q}^\ell_{\rm ph}) - \delta^{(a)}_{\boldsymbol{q}_{\rm el}}(\boldsymbol{q}^\ell_{\rm ph})\right).$$

Here, $\boldsymbol{\Psi}^{L-1}(t,\vec{\boldsymbol{q}}^{\hat{\ell}}_{\rm ph};\boldsymbol{q}_{\rm el})$ is an $L-1$ photon wave function, *conditioned* on the generic N-electron configuration, and $\vec{\boldsymbol{q}}^{\hat{\ell}}_{\rm ph}$ is an $3(L-1)$-dimensional generic configuration space position of $L-1$ photons, obtained from $\vec{\boldsymbol{q}}_{\rm ph}$ by removing $\boldsymbol{q}^\ell_{\rm ph}$.

Many photons (cont.^{d})

$\boldsymbol{\Psi}^{L-1}(t, \vec{\boldsymbol{q}}^{\hat{\ell}}_{\mathrm{ph}}; \vec{\boldsymbol{q}}_{\mathrm{el}}) \otimes_\ell \vec{\boldsymbol{v}}(t, \boldsymbol{q}_{\mathrm{el}}) \cdot \delta^{(a)}_{\vec{\boldsymbol{q}}_{\mathrm{el}}}(\boldsymbol{q}^\ell_{\mathrm{ph}})$ manifestly resembles an L-photon wave function obtained from an $(L-1)$-photon wave function, both *conditioned* on the generic N-electron configuration, by applying a "single-photon creation operator" in which $\vec{\boldsymbol{v}} \cdot \delta^{(a)}_{\vec{\boldsymbol{q}}_{\mathrm{el}}}(\boldsymbol{q}^\ell_{\mathrm{ph}})$ takes the place of the ℓ-th factor.

Many photons (cont.^{d})

Having recognized the source terms of the ♯-field equations as remnants of creation operators, it is natural to look whether there also are annihilation operators in the model. Indeed, one recognizes the "single-photon ♯-field energy"

$$E^{\sharp}(t,\vec{\boldsymbol{q}}_{\mathrm{el}}) = \frac{1}{8\pi}\int_{\mathbb{R}^3}\left(\boldsymbol{\Psi}^*\cdot\boldsymbol{\Psi}\right)(t,\boldsymbol{q}_{\mathrm{ph}};\vec{\boldsymbol{q}}_{\mathrm{el}})\mathrm{d}^3q_{\mathrm{ph}}$$

in the N-electron Schrödinger, resp. Pauli equation as a single-photon annihilation operator acting on the conditioned one-photon $\boldsymbol{\Psi}$, the "annihilation" effected by $\boldsymbol{\Psi}$ itself.
A suggestive generalization to L photons is

$$E^{\sharp}_{L}(t,\vec{\boldsymbol{q}}_{\mathrm{el}}) := \frac{1}{8\pi L}\sum_{\ell}\int_{\mathbb{R}^3}\Big(\left(\Pi_\ell\boldsymbol{\Psi}^L\right)^*\cdot\left(\Pi_\ell\boldsymbol{\Psi}^L\right)\Big)(t,\vec{\boldsymbol{q}}^{\ell}\mathrm{ph};\vec{\boldsymbol{q}}_{\mathrm{el}})\mathrm{d}^3q_{\mathrm{ph}}$$

SUMMARY

- We have developed a tentative quantum-mechanical model of electrons and photons that interact with each other and with fixed atomic nuclei.
- The model accurately reproduces all the atomic and molecular (etc.) energy spectra of the semi-relativistic so-called "standard model of everyday matter".
- It also describes the emission / absorption of EM radiation / photons by excited atoms with Rydberg–Bohr frequencies.
- The model suggests that Special Relativity may hold only as a quantum-mechanical expected "value:"
  For macroscopic phenomena, the law of large numbers would then guarantee that SR rules supreme.
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OUTLOOK

- To get to a QM whose expected value IS a truly Lorentz-covariant field theory on spacetime, Schrödinger's, respectively Pauli's equations should be replaced by a Dirac equation; e.g., for hydrogen this would be

$$\left(i\hbar\partial_0 - P_0^\sharp\right)\Psi = \boldsymbol{\alpha}\cdot\left(-i\hbar\nabla_{\boldsymbol{q}_{\rm el}} - \boldsymbol{P}^\sharp\right)\Psi + mc\beta\Psi,$$

  where the $P^\sharp$ and Ψ are functions of $(t, \boldsymbol{q}_{\rm el})$, and where $\boldsymbol{\alpha}$ and β are Dirac matrices, and Ψ is a Dirac bi-spinor.
- Also the $\sharp$ field equations, which are generalizations of the Maxwell–Lorentz field equations, should be replaced by a proper *wave equation for a photon* — see KTZ.
- The KTZ photon wave equation yields a hamiltonian with the correct photon energy $\hbar\omega = \hbar c|\boldsymbol{k}|$ and momentum $\hbar\boldsymbol{k}$.

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OUTLOOK (cont.^{d})

- A proper QM should be formulated with a single joint wave function of all these particles, not a coupled system of various partial wave functions. This joint wave function should obey a single linear wave equation.
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The Schrödinger–Maxwell ground state

For instance, the energy ground state in this model corresponds to minimizing $\mathcal{E}(\Psi, \mathbf{E}_{\rm el}, \mathbf{B}_{\rm el})$ for $\mathbf{A}_{\rm el} \equiv \mathbf{0}$ and vanishing electromagnetic radiation fields, and $\Psi(t, \mathbf{s}) = e^{-iEt/\hbar}\psi(\mathbf{s})$. We set $\mathcal{E}(e^{-iEt/\hbar}\psi, \mathbf{0}, \mathbf{0}) =: \mathcal{F}(\psi)$, thus

$$\mathcal{F}(\psi) = \int_{\mathbb{R}^3} \left(\frac{\hbar^2}{2m} |\nabla\psi|^2 - \frac{e^2}{|\mathbf{s}|} |\psi|^2 \right)(\mathbf{s}) d^3s + \frac{e^2}{2} \int_{\mathbb{R}^6} \frac{|\psi|^2(\mathbf{s}) |\psi|^2(\mathbf{s}')}{|\mathbf{s}-\mathbf{s}'|} d^3s d^3s'.$$

The functional $\mathcal{F}$ has a unique minimizer ψ_1 on the Sobolev space $H^1(\mathbb{R}^3)$ under the constraint $\int_{\mathbb{R}^3} |\psi|^2(\mathbf{s}) d^3s = 1$ [Benguria, Brezis, & Lieb]. By uniqueness it is spherically symmetric [Kawohl & Krömer]. By the virial theorem, $\mathcal{F}(\psi_1) = -\frac{\hbar^2}{2m} \int_{\mathbb{R}^3} |\nabla\psi|^2(\mathbf{s}) d^3s < 0$, as expected.

The Schrödinger–Maxwell ground state (cont.^{d})

The minimizer ψ_1 satisfies the Euler–Lagrange equation

$$-\frac{\hbar^2}{2m}\Delta_{\mathbf{s}}\psi(\mathbf{s}) - \frac{e^2}{|\mathbf{s}|}\psi(\mathbf{s}) + e^2\int_{\mathbb{R}^3}\frac{1}{|\mathbf{s}-\mathbf{s}'|}|\psi|^2(\mathbf{s}')d^3s'\psi(\mathbf{s}) = E_g\psi(\mathbf{s});$$

the eigenvalue E_g is the Lagrange multiplier for the constraint $\|\psi\|_{L^2} = 1$, [Benguria & Lieb]. The Euler-Lagrange equation is also obtained from the Schrödinger-Maxwell system, with $\Psi(t,\mathbf{s}) = e^{-iE_gt/\hbar}\psi(\mathbf{s})$, $\mathbf{A}_{\rm el} \equiv \mathbf{0}$, and $\phi_{\rm el}$ the electrostatic Coulomb potential of $\rho_{\rm el}$.
However, in this *nonlinear eigenvalue problem* the eigenvalue E_g does not coincide with the minimum of $\mathcal{F}(\psi)$.
[cf. Bazley & Seydel, 1974].

The Schrödinger–Maxwell ground state (cont.[d])

PROOF: Setting $\psi = \psi_1$ in the Euler-Lagrange equation, then multiplying it by ψ_1 and integrating over $\mathbb{R}^3$, and recalling the normalization of ψ_1, for the ground state energy E_g one obtains

$$E_g = \frac{\hbar^2}{2m}\int_{\mathbb{R}^3}|\nabla\psi_1|^2(\mathbf{s})d^3s - \int_{\mathbb{R}^3}\frac{e^2}{|\mathbf{s}|}|\psi_1|^2(\mathbf{s})d^3s + e^2\int_{\mathbb{R}^6}\frac{|\psi_1|^2(\mathbf{s})|\psi_1|^2(\mathbf{s}')}{|\mathbf{s}-\mathbf{s}'|}d^3sd^3s',$$

which is the same as

$$E_g = \mathcal{F}(\psi_1) + \frac{e^2}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|\psi_1|^2(\mathbf{s})|\psi_1|^2(\mathbf{s}')}{|\mathbf{s}-\mathbf{s}'|}d^3sd^3s'.$$

And so we have $E_g > \mathcal{F}(\psi_1)$. □

The energetic significance of E_g is obscure !

The Schrödinger–Maxwell ground state (cont.[d])

Moreover, for all non-vanishing ψ, we obviously also have

$$\mathcal{F}(\psi) > \frac{\hbar^2}{2m}\int_{\mathbb{R}^3}|\nabla\psi|^2(\mathbf{s})d^3s - \int_{\mathbb{R}^3}\frac{e^2}{|\mathbf{s}|}|\psi|^2(\mathbf{s})d^3s, \tag{38}$$

which is the usual energy functional for the QM textbook Schrödinger equation of the hydrogen eigenvalue problem in Born–Oppenheimer approximation, and so

$$\mathcal{F}(\psi_1) > E_1^{\text{Bohr}}. \tag{39}$$

So the model predicts an ionization energy $|\mathcal{F}(\psi_1)| < |E_1^{\text{Bohr}}|$.
Numerically it's off by a factor 2!