

Electronic flow and density vortices in the H₂ molecule: An analogy with the Navier–Stokes equation

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Abstract

This work proposes a deliberately analogical hydrodynamic reading of the covalent bond in the hydrogen molecule. Instead of treating the two electrons only as localized particles or as a static cloud, the electronic density is described as a continuous field that, at a modeling stage, can be visualized as a mass of water in motion. Starting from the polar decomposition of the wave function, $\psi = \sqrt{n} \exp(iS/\hbar)$, the electronic density n , probability current j , and effective velocity $v = \nabla S/m_e$ are introduced. The continuity equation and the Madelung form of quantum dynamics are then compared with the Navier–Stokes equation, with an additional force term associated with the quantum potential. The aim is not to claim that electrons are a classical fluid or that the H–H bond is literally a vortex. The central point is to show that flow language helps organize intuition about density redistribution, flux, conservation, and vortical structures. For the stationary ground state of H₂, the wave function can be chosen real and the net probability current is zero; therefore, the vortex-like flow presented here is a modeling construction for dynamical states or for the geometry of the density, rather than a permanent current predicted for the ground state.

Keywords: H₂; electronic density; electronic flow; probability current; Navier–Stokes equation; quantum hydrodynamics; vorticity; covalent bond.

1. INTRODUCTION

The bond in the hydrogen molecule is one of those problems that seems simple until we try to answer, precisely, the question “where are the electrons during bond formation?”. The conventional quantum description solves the problem very effectively: the electrons occupy a bonding molecular orbital, and the electronic density is more concentrated in the region between the two nuclei. Modern studies of H_2 also show that bond stabilization can be analyzed in terms of density redistribution and kinetic, potential, and correlation contributions [1–3].

This article proposes a change of language. Instead of imagining electronic density only as a colored surface or a motionless cloud, we ask what it would mean to describe it as if it were the surface of moving water. The comparison is intuitive: water has density, velocity, flow, pressure, viscosity, and vorticity; quantum mechanics provides probability density, current, and an effective velocity associated with the phase of the wave function. The approximation is therefore a mathematical and visual bridge, not a physical identification.

This qualification is important. The Navier–Stokes equation was developed for classical continua and relates conservation of mass, momentum, pressure, and viscosity [4]. Electrons, on the other hand, are quantum objects. What makes the comparison interesting is that the Schrödinger equation admits a hydrodynamic reformulation: writing the wave function in polar form yields a continuity equation and an equation of motion similar to Euler’s equation, but containing the so-called quantum potential [5].

The objective here is to construct a conceptual model of an “electronic vortex” for the H–H bond, making clear at each stage what is established physics, what is a mathematical analogy, and what is merely a modeling hypothesis. This separation is essential so that the image of a water current is not confused with the claim that, in the ground state of H_2 , a literal electronic liquid circulates between the atoms.

1.1. The H–H bond viewed through electronic density

In the simplest molecular treatment, the 1s orbitals of the two hydrogen atoms combine to form a bonding orbital and an antibonding orbital. In the ground state, the two electrons occupy the bonding orbital, whose amplitude is enhanced in the internuclear region [1,2]. A schematic expression for this orbital is

$$\phi_g(r) = N [1s_A(r) + 1s_B(r)]$$

and, for a two-electron state without entering the full details of electron correlation, the spatial density is proportional to $|\phi_g(r)|^2$. The result is a region of higher density between the nuclei. In the analogy proposed here, this region will be treated as the “mass” of the flowing water.

1.2. What does it mean to speak of “electronic flow”?

In quantum mechanics, the concept closest to flow is the probability current. For a wave function ψ , it can be written as

$$\mathbf{j} = (\hbar/2m_e i) [\psi^* \nabla \psi - \psi \nabla \psi^*] \quad (1)$$

and satisfies the continuity equation

$$\partial n / \partial t + \nabla \cdot \mathbf{j} = 0 \quad (2)$$

where $n = |\psi|^2$ is the probability density for one particle. For two electrons, the exact description is multidimensional and the observable electron density is obtained from the many-body wave function. Nevertheless, the local form of conservation remains a useful interpretive tool.

An important consequence is that “high density” and “high flow” are not the same thing. A spatial distribution can be highly concentrated and still have zero net current. This distinction will be decisive for interpreting the ground state of H_2 .

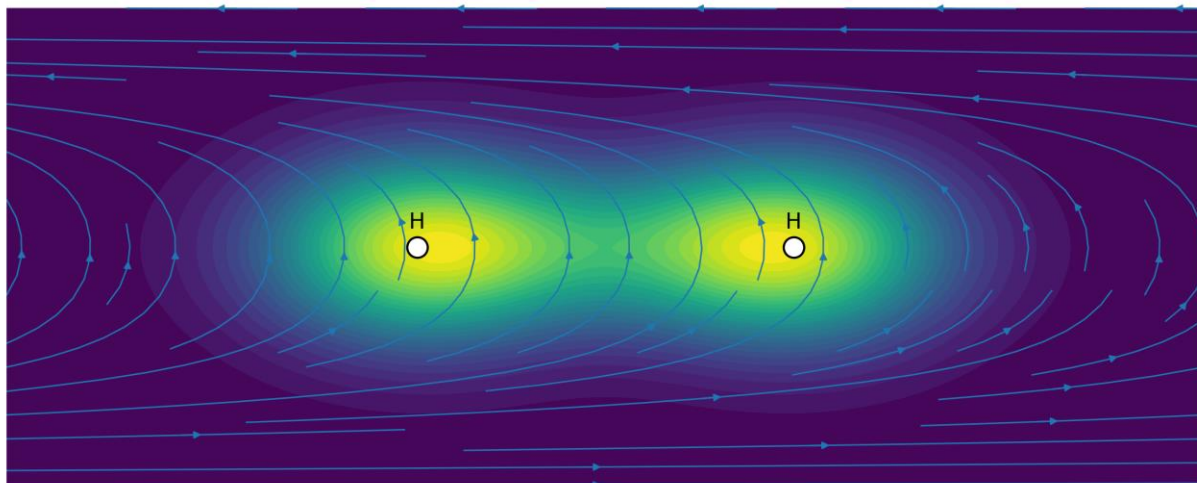


Figure 1. Schematic representation of the electron density of H_2 and of flow lines used solely as a visual aid. The figure is not an *ab initio* calculation of electron current.

2. METHODOLOGY

The study presented here is theoretical and conceptual. No experiments or high-accuracy electronic-structure calculations were performed. The methodology consists of constructing a correspondence between quantum-mechanical variables and variables in a continuum description, following four steps: (i) representing the wave function in polar form; (ii) obtaining the current and effective velocity; (iii) comparing the quantum equation of motion with Navier–Stokes; and (iv) discussing when a vortex-like image can or cannot be associated with a real electronic flow.

2.1. Polar decomposition and effective velocity

The wave function is written in Madelung form:

$$\psi(r,t) = \sqrt{n(r,t)} \exp[iS(r,t)/\hbar] \quad (3)$$

Substitution of this expression into the Schrödinger equation yields a continuity equation and a modified Hamilton–Jacobi equation. The current takes the form

$$\mathbf{j} = n\nabla S/m_e = n \mathbf{v} \quad (4)$$

which allows an effective velocity to be defined as

$$\mathbf{v} = \nabla S/m_e \quad (5)$$

This velocity should not be interpreted as the classical velocity of small “drops of electrons”. It is a variable field useful for representing quantum current. Figure 2 summarizes the correspondence between the two languages.

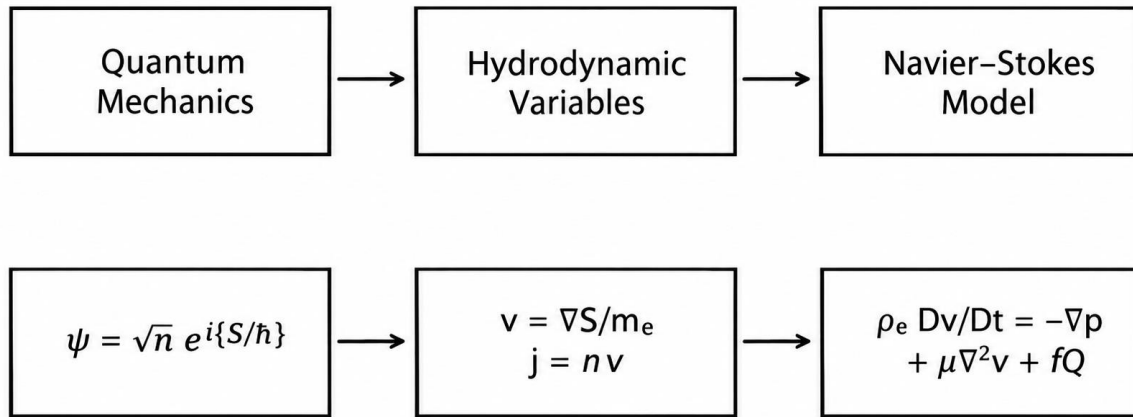


Figure 2. Conceptual correspondence between the quantum and hydrodynamic descriptions. The Navier–Stokes term is introduced as a modeling extension, not as the fundamental equation of the electron.

2.2. From the quantum equation to a hydrodynamic equation

The real part of the Schrödinger equation, after polar decomposition, leads to an equation of motion that can be written in compact form as

$$m_e [\partial \mathbf{v} / \partial t + (\mathbf{v} \cdot \nabla) \mathbf{v}] = -\nabla(V + Q) \quad (6)$$

where V represents the external potential and

$$Q = -(\hbar^2/2m_e) [\nabla^2 \sqrt{n} / \sqrt{n}] \quad (7)$$

is the quantum potential. The term Q is one of the fundamental differences between this description and classical fluid mechanics.

To approach the Navier–Stokes language, we introduce an electronic mass density $\rho_e = m_e n$ and an effective pressure p . One possible phenomenological equation is

$$\rho_e [\partial \mathbf{v} / \partial t + (\mathbf{v} \cdot \nabla) \mathbf{v}] = -\nabla p + \mu \nabla^2 \mathbf{v} + fQ \quad (8)$$

where μ is an effective viscosity, used only as a regularization or closure parameter of the model, and fQ represents the effective quantum force associated with $-\nabla Q$. The equation above should be understood as a hybrid model: the transport structure comes from fluid mechanics, while the quantum origin of the density and the Q term is preserved.

In classical fluid mechanics, the Navier–Stokes equation relates convective acceleration, pressure, viscosity, and applied forces [4]. The same mathematical pattern makes it possible to ask whether a region of electronic density can develop structures resembling streamlines, recirculation, or vorticity. The answer, however, depends on the phase of the wave function and on the dynamics under consideration.

3. RESULTS AND DISCUSSION

3.1. The Central Point: density is not flow

The comparison with water becomes clearer when three ideas are separated. The first is density: in the electronic case, $n(\mathbf{r}, t)$ indicates how the probability or electron density is distributed. The second is flow: $\mathbf{j}(\mathbf{r}, t)$ indicates the direction and intensity of the probability current. The third is vorticity. It measures, in the continuum model, the rotational character of the velocity field:

$$\boldsymbol{\omega} = \nabla \times \mathbf{v} \quad (9)$$

An electronic-density surface can have a very complex shape without any circulation. It is possible to have a “mountain” of density between the nuclei and, simultaneously, $\mathbf{j} = 0$. Therefore, drawing arrows over a density surface is a visualization choice; by itself it is not evidence of electronic motion.

3.2. The H_2 ground state and the absence of net current

For the nondegenerate ground state of an isolated molecule without external fields, the spatial wave function can be chosen real. In that case, the spatial phase is constant and the expression $\mathbf{j} = n \nabla S / m_e$ gives $\mathbf{j} = 0$. This means that the electronic density can be perfectly stable and concentrated in the bonding region without representing a permanent current of electrons around the internuclear axis.

This observation prevents a misleading interpretation of the metaphor. The “vortex” of H_2 should not be presented as a stationary current similar to a water whirlpool. What the analogy can legitimately represent is the possibility of following a temporal redistribution of density, for example during bond

formation, excitation, a superposition of states, or the action of an external field. In such cases, j can be nonzero.

3.3. Where Does the Vortex-Like Flow Enter?

Vortex-like flow appears mathematically when the velocity field has a rotational component. In a simple description based only on $v = \nabla S/m_e$, the field is irrotational in regions where S is regular, because the curl of a gradient is zero. Vortical structures can nevertheless arise in situations involving multivalued phase, nodes of the wave function, states with angular momentum, time-dependent superpositions, or extensions of the dynamics beyond the ground state.

For visualization, Figure 3 shows a generic vortical field. It does not represent the current of H_2 in its ground state. Its role is to show what the word “vortex” would mean within the model.

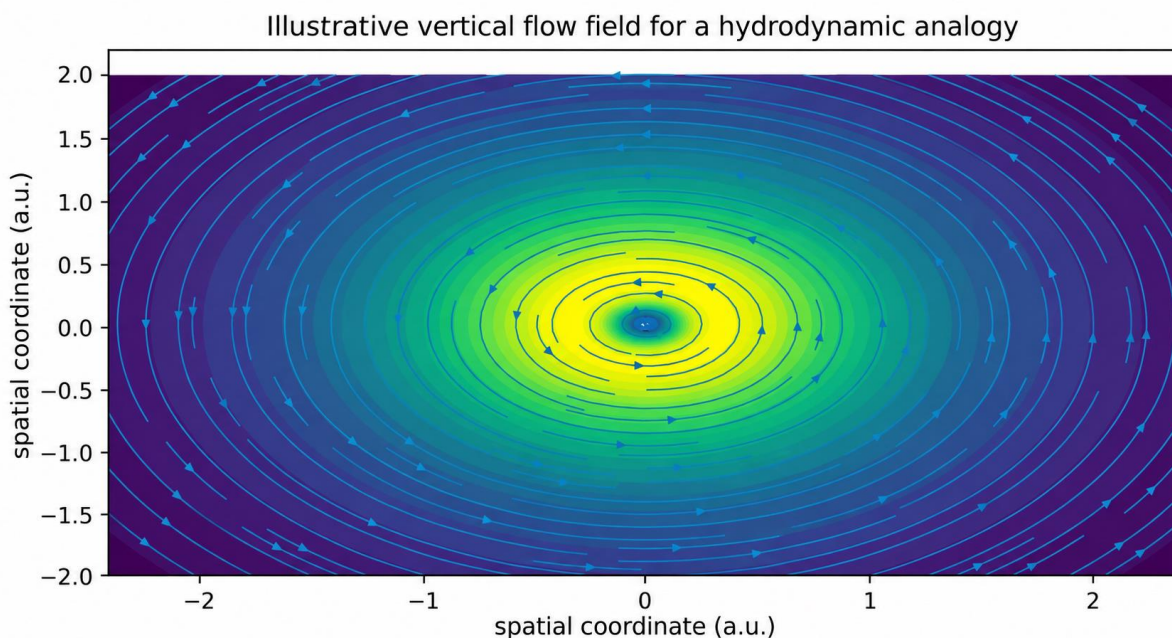


Figure 3. Generic vortical field used to illustrate the meaning of vortex-like flow in the hydrodynamic model. It does not represent a calculated current for the H_2 ground state.

3.4. A Navier–Stokes-like reading of the bond

The analogy becomes particularly interesting if we imagine a process in which two hydrogen atoms approach each other. In a classical description of water, bringing two sources closer or modifying a pressure field reorganizes the flow. In the electronic model, bringing the nuclei closer changes the Coulomb potential and, consequently, the wave function and its density.

The internuclear region can gain density because the bonding orbital combines contributions from the two centers. Table 1 summarizes the correspondence and also indicates where the analogy ceases to be literal.

Table 1. Correspondence between quantum variables and hydrodynamic variables in the proposed model.

Quantum description	Fluid analogy	Limitation
electronic density n	fluid density	not classical continuous mass
current j	mass flow	it is probability current
$v = j/n$	fluid velocity	effective velocity
$-\nabla Q$	quantum force	not an ordinary classical force
effective p	pressure	model closure parameter
$\mu \nabla^2 v$	dissipation/viscosity	does not imply material viscosity of electrons
$\omega = \nabla \times v$	vorticity	may be zero in the ground state

3.5. A parameter for measuring the “vortex”

If the goal is to transform the metaphor into a (possible) computational procedure, a measure of vortical intensity can be defined. A simple choice is the enstrophy per unit volume, proportional to

$$\mathcal{E} = 1/2 |\omega|^2 \quad (10)$$

and, in a region Ω ,

$$E\Omega = \int_{\Omega} dV \mathcal{E} \quad (11)$$

In a time-dependent calculation, it would be possible to follow $E\Omega$ while the nuclei approach one another or while an electronic superposition evolves. An increase in $E\Omega$ would mean that the effective velocity field has acquired a stronger rotational character. It would not, by itself, mean that electrons were literally “spinning like water”.

3.6. Physical interpretation: what the model can explain

The main advantage of the analogy is pedagogical and geometric. It helps us think of the bond as a region of density redistribution rather than as a simple line connecting two nuclei. It also provides a language for discussing conservation, transport, and spatial structure. This can be particularly useful when moving from H_2 to larger systems, excited states, ultrafast processes, or problems in which electronic currents are explicitly calculated.

The literature on H_2 shows that the nature of the bond can be examined through different energy and density decompositions, including contributions from delocalization and electronic redistribution [2,3]. The hydrodynamic approach does not replace these analyses. It provides an additional layer of interpretation.

3.7. Where the Model Needs Improvement

The greatest limitation lies in the viscosity term. There is no universal electronic viscosity that can simply be inserted into the Navier–Stokes equation and adjusted as if we were working with water. A more rigorous formulation would require deriving pressure and stress terms from many-body quantum

theory, or using time-dependent density functional theory, quantum hydrodynamics, or wave-packet dynamics.

A second limitation is dimensional. The observable electronic density is a function of three spatial coordinates, whereas the two-electron wave function generally depends on six spatial coordinates, in addition to spin. Therefore, any three-dimensional field $n(\mathbf{r},t)$ used in this article is a reduction of the complete information.

A third limitation is the word “turbulence”. In fluid mechanics, turbulence involves a broad hierarchy of scales, instabilities, and energy transfer. A simple vortical field is not sufficient to demonstrate turbulence. Thus, in this work, “vortex” is used in a controlled sense to mean rotational structure or recirculation of the effective field.

4. CONCLUSIONS

The hydrogen molecule provides a particularly clean setting for testing the idea of interpreting the covalent bond through hydrodynamic language. Electronic density can be treated as a continuous field for visualization purposes, while probability current provides a variable that is mathematically close to the concept of flow.

The decomposition $\psi = \sqrt{n} \exp(iS/\hbar)$ allows an effective velocity $\mathbf{v} = \nabla S/m_e$ to be defined and transforms quantum dynamics into a hydrodynamic-like form, with the quantum potential playing a role that has no counterpart in classical Navier–Stokes theory. The inclusion of pressure and viscosity terms generates a phenomenological model capable of reproducing the language of momentum transport, but these terms should not be interpreted as material properties of electrons.

The most important result is also the simplest: the electronic density of the H–H bond should not be confused with an electronic current. In the stationary ground state of H_2 , the net current can be zero even with a large density between the nuclei. Therefore, the proposed “electronic vortex” is best understood as a mathematical representation for studying transient flows, spatial phases, and rotational structures within a hydrodynamic description of the wave function.

As a perspective, a subsequent study could calculate the density and current of H_2 using time-dependent dynamics, generate vorticity maps, and compare different electronic states. This would allow a quantitative test of how far the Navier–Stokes analogy is useful and, above all, where the quantum nature of the system requires abandoning the classical fluid picture.

REFERENCES

- [1] Halpern AM. Exploring the Nature of the H_2 Bond. 1. Using Spreadsheet Calculations To Examine the Valence Bond and Molecular Orbital Methods. *J Chem Educ* 2013; 90(11): 1452–1458. doi:10.1021/ed400234g.
- [2] Graves V, Sünderhauf C, Blunt NS, et al. The Electronic Structure of the Hydrogen Molecule: A Tutorial Exercise in Classical and Quantum Computation. *ACS Phys Chem Au* 2025; 5(5): 435–449. doi:10.1021/acspyschemau.5c00030.
- [3] Wilson AK, et al. Covalent Bonding in the Hydrogen Molecule. *J Phys Chem A* 2017. doi:10.1021/acs.jpca.7b08963.
- [4] NASA Glenn Research Center. Navier-Stokes Equation. NASA; accessed 23 Sep 2026.
- [5] Madelung E. Quantentheorie in hydrodynamischer Form. *Z Phys* 1927; 40: 322–326.