

**THE ELECTRIC FIELD IN A HYDROGEN MOLECULE***Kochnev V.K.*

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Electric field and electron density in a molecule [1] are given by a solution of the Poisson differential equation for the electrostatic potential  $\phi$  subject to a set of asymptotic boundary conditions where  $\phi \sim Z/r$  for an atom of atomic number  $Z$  as  $r$  approaches zero, with a Fermi-Dirac density  $(-1) \cdot \rho$  in its right side (the charge of electrons within a volume element over the volume element itself, while adhering to the Pauli exclusion principle). Unbounded physical density (see Picture) is reminiscent of bounded probabilistic density described in Hartree-Fock theory. Energy of the field cannot be computed by integrating the energy density  $\mathbf{E} \cdot \mathbf{E} / 2$  for the tension  $\mathbf{E} = -\nabla\phi$  of the field because the integral diverges. And it cannot be computed by integrating the energy density  $(-1) \cdot \rho \cdot \phi$  until a certain value of the electrons' chemical potential  $\mu$  is assigned (both  $\rho$  and  $\phi$  depend on  $\mu$ ), which serves as the reference point for the electrostatic potential  $\phi$  (the density  $\rho$  vanishes at infinitely distant points from all nuclei, meaning by Fermi-Dirac expression that  $\phi = \mu$  is not zero at infinitely distant points). We will apply a method that has been previously used [2] for calculating the energies of atoms by solving the Poisson equation with a single asymptotic boundary condition. Namely, exclusion from calculation of an unknown expression for energy (unknown Kohn-Sham functional) by using a variationally equivalent function to get an exact value for the chemical potential of electrons to integrate  $(-1) \cdot \rho \cdot \phi$ . A binding-type curve  $E(R)$  for the hydrogen molecule is then obtained [1]. The exclusion method can be applied to arbitrary otherwise intractable potential fields [3].

1. Valentin Kochnev. The electric field in a hydrogen molecule // Journal of Mathematical Chemistry (2025, preprint). P. 1–26. <https://doi.org/10.21203/rs.3.rs-7403238/v1>

2. Kochnev, V.K. Equilibrium state energy: Atoms. Chemical Physics 517, 247–252 (2019) <https://doi.org/10.1016/j.chemphys.2018.10.018>

3. Kochnev V.K. Homogeneous functions of degree one and heat phenomena in potential fields (2024). <https://arxiv.org/abs/2401.03010>