

Density functional theory: From real to complex densities

MATTHIAS ERNZERHOF

Department of Chemistry, University of Montreal
matthias.ernzerhof@gmail.com

ABSTRACT

In density functional theory, the ground-state energy $E[\rho]$ is given in terms of the electron density ρ . The electron density for real valued wave functions is obtained as $\rho(\vec{r}) = N \int d^3r_2 d^3r_3 \dots d^3r_N \Psi(\vec{r}, \vec{r}_2, \dots, \vec{r}_N) \Psi(\vec{r}, \vec{r}_2, \dots, \vec{r}_N)$. It's noteworthy that a stationary state is an idealization, ignoring interactions with the environment, which often results in a finite lifetime of a given system. A system of finite lifetime has a complex-valued wave function and an analytic continuation of the above expression for $\rho(\vec{r})$ results in complex densities. An interesting formal question that arises is what is the interpretation of $E[\rho]$ if real electron densities are generalized by complex electron densities [1,2]? We explain that this generalization enables one to describe states of finite lifetime in addition to stationary states. We consider simple approximations to $E[\rho]$ and we analyze the energy as a functional of complex densities. We examine the corresponding solutions of the Kohn-Sham equation [1,2,3,4] and relate them to observable phenomena.

References

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