Volume Charge Density Functional Theory (VDFT)

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Abstract: Giving a path to establish the volume charge density functional theory (VDFT)

Main viewpoints and conclusions:

Volume charge density functional theory (VDFT) is a latest theory about the structure and distribution of electrons, is based on atomic concentric spherical layers-type model,[1] and is a quantum method that study the structure and distribution of multi-electrons system, the main goal of this theory is to replace the *Electron density* and the *Wave function* as basic amount of research by *Volume charge density*, finally, establish a quantum theory which meet the reality, decisive, causality, locality and completeness, multiple causes and multiple effects.

The total charge $Q = Ze^{-}$; Volume charge density functional $\rho_i = F(E, H, T, Q)$;
Frequency-field function $v = f(\rho_i) = f[F(E, H, Q, T)]$;
Energy levels represents function $E_i = hv_i = h \cdot f(\rho_i) = h \cdot \{f[F(E, H, T, Q)]\}$;
Sphere center symmetry, isotropic, $\rho_i = q_i/V_{icl}$, Distribution in the radius ρ,
Divergence on the radial gradient;
Fine Structure --- the gradient of the divergence;
Hyperfine structure --- the second gradient of the divergence;
Between the various q_i cited, balance and nuclear repulsion between.

Energy levels E_i relationship with the natural frequency v_i and the volume charge density ρ_i is:

$$E_i = hv_i = h \cdot f(\rho_i) = h \cdot \{f[F(E, H, T, Q)]\}.$$

References

[1] *Atomic concentric spherical layers-type model*
http://rxiv.org/abs/1401.0147
[2] *The Causes and Mechanism of Atomic Energy Levels Quantization*
http://vixra.org/abs/1402.0104