

Abstract Submitted
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One-to-one Correspondence of the Normalization and Coulomb Hole Sum Rules for Approximate Wave Functions.¹ XIAO-YIN PAN, VIRAH T SAHNI, LOU MASSA, The Graduate School, CUNY — For approximate wave functions, we prove the theorem that there is a one-to-one correspondence between the constraints of normalization, and of the Fermi-Coulomb and Coulomb hole sum rules. This correspondence is surprising because normalization depends on the probability of finding an electron at some position, whereas the Fermi-Coulomb/Coulomb hole sum rules depend on the probability of two electrons staying apart due to Pauli-Coulomb/Coulomb correlations. We demonstrate the theorem by example using wave function functionals². The significance of the theorem for DFT lies in the fact that the extensively employed LYP correlation energy functional³ is based on a wave function (that of Colle-Salvetti⁴) which satisfies the Coulomb hole sum rule only approximately, and that wave function is therefore not normalized.

1 Supported by RF CUNY

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Viraht Sahni
The Graduate School, CUNY

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