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Thoughts upon the approaching thirtieth anniversary of two seminal coordinate scaling papers in density functional theory

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The significance of two seminal papers on coordinate scaling in density functional theory, [Levy M & Perdew J P, *Phys Rev A*, 32 (1985) 2010 and Ghosh S K & Parr R G, *J Chem Phys*, 82 (1985) 3307] is discussed.

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In 1985, John Perdew and I published our paper in *Phys Rev A*[1], where we showed that the interacting kinetic energy, the electron-electron repulsion energy, and the correlation energy, as functionals of the electron density, satisfy inequalities upon a coordinate scaling of the density. These surprising scaling inequalities were counterintuitive because the familiar wave function theory gives equalities. In addition, we showed that the Kohn-Sham exchange functional, Ex, does exhibit a scaling equality and that Ex is equal to a simple virial-like integral involving the exchange potential and the density. This is now known as the Levy-Perdew virial relation for exchange. It enables one to obtain Ex directly from its functional derivative.

In 1985, Swapan Ghosh and Robert Parr published their paper in *J Chem Phys*[2], where they showed that any functional is equal to a simple virial-like integral involving its functional derivative (potential) and the density, if the functional satisfies a scaling equality. But they did not study the circumstances under which a functional does exhibit a scaling equality nor did they study Ex explicitly. Nevertheless, the Ghosh-Parr theorem, which they nicely proved through use of the definition of the functional derivative and the chain rule, has been quite powerful for deducing density functional identities. For instance, in 1999 Hui Ou-Yang and I derived three necessary and sufficient constraints for a potential to be the exact exchange potential[3]. The use of the Ghosh-Parr scaling theorem was crucial for the proof of our theorem. Many others have found the seductive Ghosh-Parr approach and theorem to be extremely valuable.

References

1 Levy M & Perdew J P, *Phys Rev A*, 32 (1985) 2010.
2 Ghosh S K & Parr R G, *J Chem Phys*, 82 (1985) 3307.
3 Ou-Yang H & Levy M, *Phys Rev Lett*, 65 (1990) 1036.