Further exploration of the Fukui function, hardness, and other reactivity indices and its relationships within the Kohn-Sham scheme

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The Fukui function, hardness, and other reactivity indices defined in the context of the Kohn-Sham scheme have been further examined following up previous developments. An equation analogue to the Berkowitz-Parr relationship among the noninteracting linear response function and a new Kohn-Sham softness hierarchy can be derived as defined in the present study. The thermodynamic-like structure of the mathematical equations is retained among the global, local, and nonlocal hierarchies of descriptors, yielding equations that present fewer approximations. In particular, it is stressed that the Kohn-Sham hardness is better approximated by the Kohn-Sham energy gap and, as previously emphasized, that the Kohn-Sham Fukui function is precisely equal to the square of the frontier orbital. The higher-order perturbational extensions have been outlined, and the analogue of a Fukui response function witmn the Kohn-Sham context has been derived.