Correcting models with long-range electron interaction using generalized cusp conditions

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Sources of energy errors resulting from the replacement of the physical Coulomb interaction by its long-range erfc(μ r)/r approximation are explored. It is demonstrated that the results can be dramatically improved and the range of μ giving energies within chemical accuracy limits significantly extended, if the generalized cusp conditions are used to represent the wave function at small r. The numerical results for two-electron harmonium are presented and discussed.