A New Characterization of the Chemical Bond and Heisenberg Exchange Interaction on Simple Examples

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A precise discussion of a single bond requires consideration of two-particle wave function for the particles involved. Here we define and determine rigorously the intrinsic covalency and connected characteristics on the canonical example of H_2 molecule. This is achieved by starting from analytic form for the two-particle wave function for electrons forming the bond, in which we single out the atomic contribution atomicity in an unequivocal manner.

In this way, a gradual evolution of the molecular state to its two-atomic correspondent is traced systematically with increasing interatomic distance. Analysis of the Heisenberg exchange interaction origin is detailed.

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