

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Correlated geminal wave function: a resonating valence bond approach for quantum chemistry MICHELE CASULA, CLAUDIO ATTACALITE, SANDRO SORELLA, SISSA and DEMOCRITOS National Simulation Center, Trieste, Italy — We introduce a simple correlated wave function, obtained by applying a Jastrow term to an antisymmetrized geminal power (AGP). Both the geminal and the Jastrow play a crucial role in determining its accuracy: the former permits the correct treatment of the nondynamic correlation effects, the latter allows a very rapid convergence of the geminal expansion by fulfilling the cusp conditions. The remarkable feature of this approach is that many resonating valence bonds (RVB) can be dealt simultaneously with a single determinant, at a computational cost growing with the number of electrons similarly to more conventional methods, such as Hartree-Fock or Density Functional Theory. Recently several atoms[1] and molecules[2] have been studied by using the RVB wave function; we have always obtained total energies, bonding lengths and binding energies comparable with more demanding multi configurational schemes. This ansatz opens the possibility to perform fully ab initio calculations of complex correlated molecular systems. We present preliminary results on benzene dimer and active site analogues of sulfur-iron proteins, which are still challenging compounds for quantum chemistry methods.

[1] M. Casula, S. Sorella, JCP 119, 6500 (2003)

[2] M. Casula, C. Attaccalite, S. Sorella, JCP 121, 7110 (2004)

Michele Casula

Date submitted: 01 Dec 2004

Electronic form version 1.4