

**BETHE–SALPETER CORRELATION ENERGIES OF ATOMS  
AND MOLECULES**Wim Klopper\*

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In the theoretical framework of the adiabatic-connection fluctuation–dissipation theorem, a variety of approaches will be proposed and discussed for the computation of atomic and molecular electronic correlation energies based on  $GW$  theory and the Bethe–Salpeter equation (BSE) [1].  $GW$  theory is concerned with computing the self-energy from the Green’s function  $G$  and the screened Coulomb interaction  $W$ , and an efficient implementation for computing atomic and molecular self-energies and BSE excitation energies has been reported recently [2].

When electronic correlation energies are computed in a finite basis set, it is found that the convergence of the computed atomic or molecular electronic correlation energy towards the limit of a complete, infinite basis set is very slow. In terms of the basis set’s cardinal number  $X$ , the convergence is  $X^{-3}$ , which is also found for many-body perturbation theory, the configuration interaction approach, and coupled-cluster methods. Fortunately, this slow basis-set convergence can be accelerated significantly by means of explicitly-correlated F12 methodology [3-5].

References

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