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Ultra-long-ranged dispersion interaction between degenerate molecules[1] JOHN DOBSON, Griffith Univ, ANDREAS SAVIN, CNRS, UPMC Sorbonne Universities — It is known (see e.g. [1]) that extended nano-systems with zero electronic gaps can exhibit dispersion interactions that fall off with unexpected powers of distance D. We seek to find a similar phenomenon between finite molecules that have a strictly degenerate many-electron groundstate (zero gap). As a toy model we take H_3 with the atoms constrained to lie on an equilateral triangle of side a, using a minimal (s) basis set, and with spin-orbit coupling omitted. Rotational symmetry at fixed spins guarantees a degenerate time-reversed pair of three-electron states. For sufficiently small atomic spacing a where inter-atomic hopping kinetic energy dominates the electron-electron repulsion, these degenerate time-reversed pairs of states are many-electron groundstates. We confirm this groundstate degeneracy via limited-basis CI calculations. We show that the resulting dispersion energy between two such constrained H_3 molecules falls off as D^{**}(-3)instead of the usual *D**(-6)*. Within the classification scheme proposed in ref [2], this effect can be interpreted as a "type C non-additivity" of the dispersion interaction. This model may be relevant to metal atom clusters.

[1] John F. Dobson, Angela White and Angel Rubio, Phys. Rev. Lett. **96** (2006) 073201.
[2] John F. Dobson, Int. J. Quantum Chem. 114, 1157 (2014).

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