

# Does Direct Perturbation Theory converge?

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Direct Perturbation Theory (DPT) is an elegant approach to treat relativistic effects in a perturbative manner. The basic idea behind DPT is to change the metric in the Dirac equation and then to employ a perturbative expansion in powers of  $c^{-2}$  with  $c$  as the speed of light. This expansion gives the correct non-relativistic limit and is in principle applicable in any order.

Implementation of DPT is facilitated if the theory is formulated in terms of energy derivatives using the method of Lagrange multipliers. In this manner, analytic derivative techniques can be exploited.

However, for any perturbative method to become a reliable tool, convergence needs to be ensured. Kutzelnigg showed that DPT converges for hydrogen-like atoms up until the nuclear charge of  $Z = 137$  [1]. To which degree this behaviour is generalizable to atoms and molecules with more than one electron will be discussed for Hartree-Fock as well as for correlated methods.

Furthermore, a simplified "one-electron" variant of lowest-order DPT (DPT2-1e) which does not require relativistic two-electron integrals is introduced and its performance is investigated.

[1] Kutzelnigg, W. *Z. Phys. D.*, 11:5-28, 1989.