Perturbation Theory for Constrained Electron Transfer

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As an alternative to the constrained density functional theory (CDFT) proposed by Wu and Van Voorhis [1], in this work, a perturbation theory is developed to describe a constrained electron transfer in a system. Perturbation theory is applied to modify the ground state density of the system with the perturbed density, to describe the system with the constrained charge transferred. The perturbed densities are obtained through auxiliary density perturbation theory (ADPT) [4], which implies, that this trial implementation in deMon2k is as efficient as the current implementation for response properties. We compare our results with respect to the ones obtained with CDFT.

References:

1. Q. Wu, T. Van Voorhis, *Phys. Rev. A* **72**, 024502 (2005).
2. R. Flores-Moreno, J. Carmona-Espíndola, A. M. Köster, *AIP Conference Proceedings* **1642,**60 (2015).