# First-order properties of ionized states from local coupled cluster response theory with density fitting

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**Abstract**

Linear response (LR) theory offers an approach for approximate coupled cluster (CC) models, like CC2 or CC3, to treat electronically excited and ionized states in a well defined way.

Wälz *et al.*[1] presented a hierarchy of local coupled cluster singles and doubles response methods for ionization potentials (IPs). The order with respect to the fluctuation potential of the IP-CC2 LR Jacobian was systematically extended up to IP-CCSD LR, while the accuracy of the ground state amplitudes were kept at the level of CC2 or MP2.

Based on this approach, analytic first-order properties for local IP-CC2 LR were implemented. Higher-order corrections according to the hierarchical scheme were calculated numerically, using a finite-field approach. Results were compared to a reference in the equation-of-motion (EOM) CC framework, namely EOMIP-CCSD on top of a CCSD ground state calculation. The main motivation is not the computation of properties *per se*, but to make a further step towards efficient analytic nuclear gradients for ionized states. Derivation and implementation of orbital-relaxation within the local IP-CC2 LR framework is presently under way.

**Keywords**

Local correlation methods, ionized state, linear response theory, finite-field calculations, analytic gradients

**References**

[1] G. Wälz, D. Usvyat, T. Korona and M. Schütz, J. Chem. Phys. **144**, 084117 (2016).