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Optimization of constrained density functional theory

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Constrained density functional theory (cDFT) is a versatile electronic structure method enabling ground-state calculations to be performed subject to physical constraints, broadening their applicability and utility. Automated optimisation of Lagrange multipliers is necessary for multiple constraints to be applied efficiently in cDFT, and for it to be applied in tandem with geometry optimization or molecular dynamics. In order to facilitate this, we provide a detailed treatment of the possible character and uniqueness of cDFT stationary points. We calculate the relevant derivatives with a new emphasis on the roles played by Kohn Sham orbital orthonormality, electronic interactions and screening described by the microscopic dielectric function. New, generally applicable expressions are derived, which relate the second-derivatives of the total-energy, its constraint and constraint-free components, to integrated response and inverse response functions. Formulae are constructed for building gradient preconditioners for cDFT, and for use with root-finding algorithms related to Newton's method, while circumventing explicit summation over unoccupied states.

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