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Constrained Density Functional Theory by Imaginary Time-Step Method DANIEL KIDD, Vanderbilt University — Constrained Density Functional Theory (CDFT) has been a popular choice within the last decade for sidestepping the self interaction problem within long-range charge transfer calculations.[1] Typically an inner constraint loop is added within the self-consistent field iterations of DFT in order to enforce this charge transfer state by means of a Lagrange multiplier method.[2] In this work, an alternate implementation of CDFT is introduced, that of the imaginary time-step method, which lends itself more readily to real space calculations in the ability to solve numerically for 3D local external potentials which enforce arbitrary given densities. This method has been shown to reproduce the proper $1/R$ dependence of charge transfer systems in real space calculations as well as the ability to generate useful constraint potentials. As an example application, this method is shown to be capable of describing defects within periodic systems using finite calculations by constraining the 3D density to that of the periodically calculated perfect system at the boundaries.

[1]Q. Wu and T. Voorhis, **J. Chem. Theory Comput.** 2, 765-774 (2006).
[2]Q. Wu and T. Voorhis, **Phy. Rev. A** 72, 024502 (2005).

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